

#### Quantum field-theoretic machine learning

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Joint work with Profs. Gert Aarts and Biagio Lucini.

# Can we view machine learning as part of quantum field theory?

And why?

#### Probability distribution

A probability distribution is a product of strictly positive and appropriately normalized factors (or potential functions) ψ:

$$p(\phi) = \frac{\prod_{c \in C} \psi_c(\phi)}{\int_{\phi} \prod_{c \in C} \psi_c(\phi) d\phi},$$

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1. Factors are the fundamental building blocks of probability distributions.

2. By controlling the factors we are able to control the form of the probability distribution.

We require some form of representation to construct the probability distribution. We are going to use a finite set  $\Lambda$  that we express as a graph  $\mathcal{G}(\Lambda, e)$  where e is the set of edges in  $\mathcal{G}$ .

A clique c is a subset of  $\Lambda$  where the points are pairwise connected. A maximal clique is a clique where we cannot add another point that is pairwise connected with <u>all</u> the points in the subset.

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There are only two maximal cliques, the subsets {A,B,C} and {C,D}.

{A,B} is a clique but it is **not** maximal because another point (C) can be included that is pairwise connected with both {A,B}.

{A,B,C,D} is **not** a clique and **not** maximal because (D) is not pairwise connected with all other points (and vice versa).



On the square lattice a maximal clique is a link.



# On a triangular lattice a maximal clique is a triangle.



On the square lattice with both diagonals a maximal clique is a square.



On the bipartite graph, which represents conventional neural network architectures a maximal clique is a link. Given a graph  $\mathcal{G}(\Lambda, e)$ , the random variables  $\varphi_i$  at each point i define a Markov random field if they fulfill the local Markov property with respect to  $\mathcal{G}$ .

The local Markov property denotes that a random variable  $\phi_i$  depends only on its neighbors and it is conditionally independent of all other random variables in the set:



$$p(\phi_i|(\phi_j)_{j\in\Lambda-\phi_i}) = p(\phi_i|(\phi_j)_{j\in\Lambda_i}).$$

#### Hammersley-Clifford theorem

A strictly positive distribution p satisfies the local Markov property of an undirected graph  $\mathcal{G}$ , if and only if p can be represented as a product of strictly positive potential functions  $\psi_c$  over  $\mathcal{G}$ , one per maximal clique c, i.e.

$$p(\phi) = \frac{1}{Z} \prod_{c \in C} \psi_c(\phi), \quad Z = \int_{\phi} \prod_{c \in C} \psi_c(\phi) d\phi$$

where Z is the partition function and  $\phi$  are all possible states of the system.

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- 1. We can devise potential functions that satisfy the Hammersley-Clifford theorem to construct a Markov random field.
- We can evaluate if known physical systems can be recast within this mathematical framework by verifying instead if they satisfy the theorem.
  We will pursue the second direction.

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### $2d \phi^4$ theory:

$$\begin{split} \mathcal{L}_E &= \frac{\kappa}{2} (\nabla \phi)^2 + \frac{\mu_0^2}{2} \phi^2 + \frac{\lambda}{4} \phi^4, \\ S_E &= -\kappa_L \sum_{\langle ij \rangle} \phi_i \phi_j + \frac{(\mu_L^2 + 4\kappa_L)}{2} \sum_i \phi_i^2 + \frac{\lambda_L}{4} \sum_i \phi_i^4. \\ \mathbf{k}_{\mathrm{L}}, \mu_{\mathrm{L}}, \lambda_{\mathrm{L}} \text{ dimensionless parameters} \end{split}$$

$$w = \kappa_L, \ a = (\mu_L^2 + 4\kappa_L)/2, \ b = \lambda_L/4$$

### Inhomogeneous $\phi^4$ theory:

$$S(\phi;\theta) = -\sum_{\langle ij \rangle} w_{ij}\phi_i\phi_j + \sum_i a_i\phi_i^2 + \sum_i b_i\phi_i^4,$$



The  $\phi^4$  theory is formulated on a square lattice which is equivalent to a graph  $\mathcal{G}(\Lambda, e)$ where  $\Lambda$  is the set of lattice sites and e the links. A non-unique choice of potential function per each maximal clique is:

$$\psi_{c} = \exp\left[-w_{ij}\phi_{i}\phi_{j} + \frac{1}{4}(a_{i}\phi_{i}^{2} + a_{j}\phi_{j}^{2} + b_{i}\phi_{i}^{4} + b_{j}\phi_{j}^{4})\right],$$

The probability distribution is expressed as a product of strictly positive potential functions  $\psi$ , over each maximal clique:

$$p(\phi;\theta) = \frac{\exp\left[\sum_{c \in C} \ln \psi_c(\phi)\right]}{\int_{\phi} \exp\left[\sum_{c \in C} \ln \psi_c(\phi)\right] d\phi} = \frac{1}{Z} \prod_{c \in C} \psi_c(\phi).$$

The  $\phi^4$  theory satisfies Markov properties and it is therefore a Markov random field.

The Markov property in a Markov chain



The Markov property in a Markov chain



The Markov property in a Markov chain



A Markov random field satisfies the Markov property in high-dimensions



# Having established that certain physical systems are Markov random fields, how do we use them for machine learning?

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Exactly in the same way as any other machine learning algorithm...

The  $\phi^4$  theory has a probability distribution  $p(\phi; \theta)$  with action  $S(\phi; \theta)$ :

$$p(\phi; \theta) = \frac{\exp\left[-S(\phi; \theta)\right]}{\int_{\phi} \exp[-S(\phi, \theta)] d\phi}$$

We now consider a different statistical system or quantum field theory with action or Hamiltonian A and a target probability distribution  $q(\phi)$ :

$$q(\phi) = \exp[-\mathcal{A}]/Z_{\mathcal{A}}$$

We can then define an asymmetric distance between the probability distributions  $p(\phi;\theta)$  and  $q(\phi)$ , which is called the Kullback-Leibler divergence:

$$KL(p||q) = \int_{-\infty}^{\infty} p(\boldsymbol{\phi}; \theta) \ln \frac{p(\boldsymbol{\phi}; \theta)}{q(\boldsymbol{\phi})} d\boldsymbol{\phi} \ge 0.$$

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We want to minimize the Kullback-Leibler divergence.

By minimizing it we would make the two probability distributions equal. We can then use the probability distribution  $p(\phi;\theta)$  to draw samples from the target distribution  $q(\phi)$ . In essence after the minimization we have created a mapping between the probability distributions of the two systems.

We now substitute the two probability distributions in the Kullback-Leibler divergence to obtain:

$$F_{\mathcal{A}} \leq \langle \mathcal{A} - S \rangle_{p(\phi;\theta)} + F \equiv \mathcal{F},$$

The expression above sets a rigorous upper bound to the calculation of the free energy of the system with action A and this calculation is conducted entirely on samples drawn from the distribution  $p(\phi;\theta)$  of the  $\phi^4$  theory.

To minimize the variational free energy we implement a gradient-based approach:

$$\frac{\partial \mathcal{F}}{\partial \theta_i} = \langle \mathcal{A} \rangle \Big\langle \frac{\partial S}{\partial \theta_i} \Big\rangle - \Big\langle \mathcal{A} \frac{\partial S}{\partial \theta_i} \Big\rangle + \Big\langle S \frac{\partial S}{\partial \theta_i} \Big\rangle - \langle S \rangle \Big\langle \frac{\partial S}{\partial \theta_i} \Big\rangle,$$

We then update the coupling constants  $\theta$  at each step t until convergence.

$$\theta^{(t+1)} = \theta^{(t)} - \eta * \mathcal{L}, \quad \mathcal{L} = \partial \mathcal{F} / \partial \theta^{(t)}$$

After training we expect that, practically:

$$\mathcal{F} \approx F_A \qquad p(\phi; \theta) \approx q(\phi).$$

A proof-of-principle demonstration is to use the inhomogeneous action S:

$$S(\phi;\theta) = -\sum_{\langle ij\rangle} w_{ij}\phi_i\phi_j + \sum_i a_i\phi_i^2 + \sum_i b_i\phi_i^4,$$

to learn an action that includes longer-range interactions:

$$\mathcal{A}_{\{4\}}(\phi) = -\sum_{\langle ij \rangle} \phi_i \phi_j + 1.52425 \sum_i \phi_i^2 + 0.175 \sum_i \phi_i^4 - \sum_{\langle ij \rangle_{nnn}} \phi_i \phi_j$$



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to learn an action that includes longer-range interactions:



What does the approximate equality of two probability distributions imply?

 $p(\phi; \theta) \approx q(\phi),$ 

We anticipate that observables calculated under the ensembles will also be approximately equal.

 $\langle O \rangle_{p(\phi;\theta)} \approx \langle O \rangle_{q(\phi)}.$ 

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$$\langle O \rangle_{p(\phi;\theta)} \approx \langle O \rangle_{q(\phi)}.$$

The numerical estimator/expectation value of an arbitrary observable O during a Monte Carlo simulation:

$$\langle O \rangle_{q(\phi)} = \frac{\sum_{l=1}^{N} \tilde{p}_{l}^{-1} O_{l} \exp[-\sum_{k=1}^{4} g_{k} \mathcal{A}_{l}^{(k)}]}{\sum_{l=1}^{N} \tilde{p}_{l}^{-1} \exp[-\sum_{k=1}^{4} g_{k} \mathcal{A}_{l}^{(k)}]},$$

Three reweighting (simultaneous) steps: Make the (already trained) inhomogeneous action S:

$$S(\phi;\theta) = -\sum_{\langle ij\rangle} w_{ij}\phi_i\phi_j + \sum_i a_i\phi_i^2 + \sum_i b_i\phi_i^4,$$

Equal to the target action A (acts as a correction step):

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Extrapolate in the parameter space along the trajectory of a coupling constant g' of A

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Simply put, an inhomogeneous system can approximate target distributions better than what the same homogeneous system can.

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$$S(\phi;\theta) = -\sum_{\langle ij \rangle} w_{ij}\phi_i\phi_j + \sum_i a_i\phi_i^2 + \sum_i b_i\phi_i^4,$$
$$S(\phi;\theta) = -w\sum_{\langle ij \rangle} \phi_i\phi_j + a\sum_i \phi_i^2 + b\sum_i \phi_i^4$$

#### **Neural Networks**

#### $\phi^4$ Markov random field





#### $\phi^4$ neural network



Hidden layer

Visible layer

$$S(\phi, h; \theta) = -\sum_{i,j} w_{ij}\phi_i h_j + \sum_i r_i \phi_i + \sum_i a_i \phi_i^2$$
$$+ \sum_i b_i \phi_i^4 + \sum_j s_j h_j + \sum_j m_j h_j^2 + \sum_j n_j h_j^4,$$
$$\theta = \{w_{ij}, r_i, a_i, b_i, s_j, m_j, n_j\}$$
$$p(\phi, h; \theta) = \frac{\exp[-S(\phi, h; \theta)]}{\int_{\phi, h} \exp[-S(\phi, h; \theta)] d\phi dh}.$$

#### **Neural Networks**

#### The $\phi^4$ neural network:

$$S(\phi, h; \theta) = -\sum_{i,j} w_{ij} \phi_i h_j + \sum_i r_i \phi_i + \sum_i a_i \phi_i^2 + \sum_i b_i \phi_i^4 + \sum_j s_j h_j + \sum_j m_j h_j^2 + \sum_j n_j h_j^4,$$

is a generalization of other neural network architectures:



 $\phi^4$  equivalence with the Ising model (under an appropriate limit)

The same approach can be used even when the probability distribution is not known, but we have the probability distribution encoded in some available data. The data can be anything: images or experimental data or a set of Monte Carlo configurations.

$$KL(q||p) = \int_{-\infty}^{\infty} q(\boldsymbol{\phi}) \ln \frac{q(\boldsymbol{\phi})}{p(\boldsymbol{\phi};\theta)} d\boldsymbol{\phi}.$$











Can we view machine learning functions as statistical-mechanical observables (in a somewhat formal manner)?

Training of a neural network on the Ising model:

Labeled as 1.









The **configuration** is drawn from an equilibrium distribution and therefore has an **associated Boltzmann weight**.

The **output** is calculated on the configuration so it must have the **same Boltzmann weight**.

# The neural network function is an observable in the system:

$$\langle f \rangle = \sum_{\sigma} f_{\sigma} p_{\sigma} = \frac{\sum_{\sigma} f_{\sigma} \exp[-\beta E_{\sigma}]}{\sum_{\sigma} \exp[-\beta E_{\sigma}]}$$

 $\sigma$  : configuration of the system

 $p_{\sigma}$  : Boltzmann probability distribution

 $\beta$ : inverse temperature





Results obtained by quantities derived entirely from the neural network

The function  $f(\cdot)$  was learned on configurations of the Ising model and f(x) can successfully predict the phase of Ising configurations x.

But what happens if we give configurations x' of a different system as input to the Ising-learned function f(·)? Can we accurately separate phases in different systems? Can we discover a phase transition through f(x')?



Mapping distinct phase transitions to a neural network, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. E 102, 053306 (2020).

Potts models:



#### Results obtained through a function f learned exclusively on the Ising model.

Mapping distinct phase transitions to a neural network, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. E 102, 053306 (2020).

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 $\varphi^4$  scalar field theory:



Fixed dimensionless  $\lambda$ =0.7 and varied the dimensionless mass  $\mu^2$ 

#### Results obtained through a function f learned exclusively on the Ising model.

Mapping distinct phase transitions to a neural network, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. E 102, 053306 (2020).



TABLE II. Critical  $\mu_c^2$  for fixed  $\lambda_L = 0.7$  and critical exponents of the  $\phi^4$  scalar field theory.

# The neural network function f is an observable in the system.

# But what does this mean?

Parameters, constraints or fields that interact with a system have conjugate variables which represent the response of the system to the perturbation of the corresponding parameter.

Can we make the same statement about the neural network function f?

We considered that Vf, where V is the volume of the system, couples to an arbitrary external field Y and defined a modified Hamiltonian for the Ising model:

$$E_Y = E - V f Y$$

We considered that Vf, where V is the volume of the system, couples to an arbitrary external field Y and defined a modified Hamiltonian for the Ising model:

$$E_Y = E - V f Y.$$

#### The question:

What happens if we allow a statistical system to interact with a neural network that has been trained to accurately separate its phases? The external field Y denotes the strength of the interaction.

Expectation value of an arbitrary observable <O> during a Monte Carlo simulation in the modified system:

$$\langle O \rangle = \frac{\sum_{i=1}^{N} O_{\sigma_i} \tilde{p}_{\sigma_i}^{-1} \exp[-\beta E_{\sigma_i} + \beta V f_{\sigma_i} Y]}{\sum_{i=1}^{N} \tilde{p}_{\sigma_i}^{-1} \exp[-\beta E_{\sigma_i} + \beta V f_{\sigma_i} Y]}$$

By choosing  $\tilde{p}_{\sigma_i}$  equal to the probabilities of the original system:

$$\langle O \rangle = \frac{\sum_{i=1}^{N} O_{\sigma_i} \exp[\beta V f_{\sigma_i} Y]}{\sum_{i=1}^{N} \exp[\beta V f_{\sigma_i} Y]}$$

#### This form of reweighting is Hamiltonian-agnostic.



FIG. 2. Mean neural network function  $\langle f \rangle$  versus external field Y at inverse temperature  $\beta = 0.43, 0, 440687, 0.45$  (right to left). The statistical uncertainty is comparable with the width of the lines. Recall that:

 $\beta$ =0.43-> symmetric phase

 $\beta_{c}$  = 0.440687 -> inverse critical temperature

 $\beta$ =0.45-> broken-symmetry phase



FIG. 3. Mean susceptibility of the neural network function  $\langle \chi_f \rangle$  versus external field Y at inverse temperature  $\beta = 0.43, 0, 440687, 0.45$  (right to left). The statistical uncertainty is comparable with the width of the lines.

#### Renormalization Group in Real Space

We then studied the neural network function f within the framework of the renormalization group and we were able to obtain the two relevant operators v and  $\theta$  that govern the divergence of the correlation length in the Ising model as well as its critical point  $\beta_c$ .



$$\beta_c = 0.44063(21)$$
  $\nu = 1.01(2)$   $\theta_Y = 0.534(3)$ 

#### For machine learning in phase transitions:

- 1. No knowledge about the order parameter is required. Effective order parameters can be constructed for systems that undergo distinct phase transitions (universality class, order, etc.).
- 2. Machine learning observables can be extrapolated or interpolated in parameter space with reweighting. This can additionally be achieved with Hamiltonian-agnostic reweighting.
- 3. Neural networks can be included in Hamiltonians/lattice actions to break or restore symmetries.
- 4. We can obtain multiple critical exponents with machine learning functions.

#### For quantum field-theoretic machine learning:

All one needs to conduct machine learning is any probability distribution  $p(\phi; \theta)$ :

$$KL(q||p) = \int_{-\infty}^{\infty} q(\boldsymbol{\phi}) \ln \frac{q(\boldsymbol{\phi})}{p(\boldsymbol{\phi};\theta)} d\boldsymbol{\phi}.$$

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Why do we ensure that the Markov property is satisfied?

# If we view machine learning as a physical concept...

... is lattice field theory the appropriate tool to describe it?

# The Lattice is...

1. Mathematical.

#### A (mathematically rigorous) bridge between Euclidean and Minkowski QFT:

Construction of quantum fields from Markoff fields, E. Nelson, J. Funct. Anal. 12, 97 (1973)

# The Lattice is...

- 1. Mathematical.
- 2. Theoretical.

#### The physics of inhomogeneous quantum field theories:

Renormalization Group in Field Theories with Quantum Quenched Disorder, V. Narovlansky and O. Aharony, Phys. Rev. Lett. 121, 071601 (2018) Renormalization group flow in field theories with quenched disorder, O. Aharony and V. Narovlansky, Phys. Rev. D 104398, 045012 (2018). Disorder in large-*N* theories, O. Aharony, Z. Komargodski, & S. Yankielowicz, J. High Energ. Phys. **2016**, 13 (2016).

# The Lattice is...

- 1. Mathematical.
- 2. Theoretical.
- 3. Experimental.

#### An interesting read:

The Hintons in your Neural Network: a Quantum Field Theory View of Deep Learning, Roberto Bondesan, Max Welling, arXiv:2103.04913.

# The Lattice is...

- 1. Mathematical.
- 2. Theoretical.
- 3. Experimental.
- 4. Computational.

# The Lattice is...

- 1. Mathematical.
- 2. Theoretical.
- 3. Experimental.
- 4. Computational.

### Thank you for your attention!

Quantum field-theoretic machine learning, D. Bachtis, G. Aarts and B. Lucini, (arXiv:2102.09449), Phys. Rev. D 103, 074510. Adding machine learning within Hamiltonians: Renormalization group transformations, symmetry breaking and restoration, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. Research 3, 013134 (2020). Mapping distinct phase transitions to a neural network, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. E 102, 053306 (2020). Extending machine learning classification capabilities with histogram reweighting, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. E 102, 053306 (2020).



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#### EuroPLEx

European network for Particle physics, Lattice field theory and Extreme computing