Disorder, phase transitions, and (lattice) quantum field-theoretic machine learning

Dimitrios Bachtis

Outline:

• Disorder

What are the connections between machine learning and disordered systems?

Prototypical types of disorder/inhomogeneity, Ising model, Ising spin glass, Ising random field, the ϕ^4 spin glass, replica theory and the overlap order parameter, intuitive connections with machine learning.

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• Quantum field-theoretic (and statistical-mechanical) machine learning How can we unify statistical mechanics, quantum field theory, and machine learning under a common mathematical framework?

The (local) Markov property, Hammersley-Clifford theorem, Nelson construction of quantum field theories, ϕ^4 Markov fields, ϕ^4 multi-agent systems, reinforcement learning, ϕ^4 neural networks and their generalization of the Bernoulli-Bernoulli restricted Boltzmann machine [see Nobel Prize 2024 (Hinton)], applications.

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• Phase transitions of machine learning algorithms

Are there ***genuine*** phase transitions in neural networks?

Second-order phase transitions during the learning process of neural networks, order parameters, scaling and universality in probabilistic machine learning, a quest for unification of machine learning under universality classes, numerical examples.



$$H = -J\sum_{\langle ij\rangle} s_i s_j$$

Z₂ or Reflection symmetry

s_i -> -s_i



$$H = -J\sum_{\langle ij\rangle} s_i s_j$$

Z₂ Symmetric phase



Critical region



Broken Z₂ symmetry phase



$$H = -J\sum_{\langle ij\rangle} s_i s_j$$

Explicit breaking of the Z₂ symmetry via a magnetic field

$$H=-J\sum_{\langle ij
angle}s_is_j-h\sum_is_i$$

Broken symmetry phase



The random field Ising model

$$H = -J\sum_{\langle ij\rangle} s_i s_j - \sum_i h_i s_i$$



The random field Ising model

$$H = -J\sum_{\langle ij\rangle} s_i s_j - \sum_i h_i s_i$$



Random Magnetic Fields, Supersymmetry, and Negative Dimensions, G. Parisi, N. Sourlas, Phys. Rev. Lett. 43, 744, (1979).

Parisi-Sourlas Supersymmetry in Random Field Models, A. Kaviraj, S. Rychkov, E. Trevisani, Phys. Rev. Lett. 129, 045701, (2022).

The Ising spin glass (the Edwards-Anderson model)

$$H = -\sum_{\langle ij\rangle} J_{ij} s_i s_j$$



The Ising spin glass (the Edwards-Anderson model)

$$H = -\sum_{\langle ij\rangle} J_{ij} s_i s_j$$

Symmetric phase

Broken symmetry phase

Evolving randomly oriented configurations



Frozen randomly oriented configuration



The Ising spin glass satisfies gauge invariance properties. For every nonzero function f:

 $s'_i \to f_i s_i \qquad J'_{ij} \to f_i^{-1} J_{ij} f_j^{-1}$

The Ising spin glass

Real replicas

$$H_{\sigma, au} = H_\sigma + H_ au = -\sum_{\langle ij
angle} J_{ij}(s_is_j + t_it_j)$$





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Overlap variable

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The ϕ^4 glass

$$S_{\Phi} = -\sum_{\langle ij \rangle} J_{ij} \phi_i \phi_j + \left(d + \frac{\mu^2}{2}\right) \sum_i \phi_i^2 + \frac{\lambda}{4} \sum_i \phi_i^4$$

Disordered Lattice Glass ϕ^4 Quantum Field Theory , D. Bachtis, arxiv2407.06569.

The ϕ^4 glass



Disordered Lattice Glass ϕ^4 Quantum Field Theory , D. Bachtis, arxiv2407.06569.

The ϕ^4 glass



Proof that the ϕ^4 spin glass reduces to the Edwards-Anderson model

$$Z_{\Phi} < \left[\int_{-\infty}^{\infty} \exp\left[-\left(\frac{\mu^2}{2}\phi_i^2 + \frac{\lambda}{4}\phi_i^4\right) \right] d\phi_i \right]^V < \infty$$
$$\lim_{\lambda \to \infty} \frac{\sqrt{\lambda}}{\sqrt{\pi}} \exp\left[-\lambda(\phi^2 - 1)^2 \right] = \delta(\phi^2 - 1)$$

Disordered Lattice Glass \$\$\phi^4\$ Quantum Field Theory , D. Bachtis, arxiv2407.06569.

Disordered systems and machine learning

Why neural networks resemble disordered systems?

The random field Ising model

$$H = -J\sum_{\langle ij\rangle} s_i s_j - \sum_i h_i s_i$$

The Ising spin glass

$$H = -\sum_{\langle ij\rangle} J_{ij} s_i s_j$$

The random field Ising model

The Ising spin glass

$$H = -J\sum_{\langle ij\rangle} s_i s_j - \sum_i h_i s_i \qquad \qquad H = -\sum_{\langle ij\rangle} J_{ij} s_i s_j$$

Neural networks, e.g. the restricted Boltzmann machine, have a Hamiltonian that looks like this:

$$H = -\sum_{i,j} w_{ij} u_i h_j - \sum_i a_i u_i - \sum_j b_j h_j$$



How can we unify statistical mechanics, quantum field theory, and machine learning under a common mathematical framework?

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



A clique c is a subset of Λ 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.

On the square lattice a maximal clique is a two-site edge.



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 standard neural network architectures a maximal clique is defined by an edge connection.

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 probability distribution.

Factorization of probability distributions



Factorization of probability distributions



Factorization of probability distributions

$$H=-\sum_{\langle ij
angle} s_i s_j \ \psi_1 = \exp[s_1 s_2 + s_1 s_3] \ \psi_1 = \sum_{\substack{\langle ij
angle}} s_1 s_2 + s_1 s_3] \ \psi_2 = \exp[s_2 s_4 + s_3 s_4] \ \psi_2 = \exp[s_2 s_4 + s_3 s_4] \ \psi_2$$

 $\sum \psi_1 \psi_2$

Hammersley-Clifford theorem

A strictly positive distribution p satisfies the local Markov property of an undirected graph *G*:

$$p(\phi_i|(\phi_j)_{j\in\Lambda-i}) = p(\phi_i|(\phi_j)_{j\in\mathcal{N}_i})$$

if and only if p can be represented as a product of strictly positive potential functions ψ_c over *G*, <u>one per maximal clique</u> 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 ϕ are all possible states of the system.

The ϕ^4 lattice field theory is, by definition, formulated on a square lattice which is equivalent to a graph $G(\Lambda, e)$. A non-unique choice of potential function per each maximal clique is:

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



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

The ϕ^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



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



Representation

Hammersley-Clifford theorem

Markov fields on finite graphs and lattices, J. M. Hammersley, P. Clifford, (1971).

Proofs

- 1) A theorem about random fields, G. R. Grimmett, Bulletin of the London Mathematical Society, 5 (1): 81–84 (1973).
- Generalized Gibbs states and Markov random fields, C. J. Preston, Advances in Applied Probability, 5 (2): 242–261, (1973).
- 3) Markov random fields and Gibbs random fields, S. Sherman, Israel Journal of Mathematics, 14 (1): 92–103, (1973).
- 4) Spatial interaction and the statistical analysis of lattice systems, J. Besag, Journal of the Royal Statistical Society, Series B, 36 (2): 192–236,, (1974).

Representation

Constructive field theory (see also J. Halverson talks!)

based on Garding-Wightman

Markov Property

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

Reflection Positivity

Reflection Positivity Then and Now, A. Jaffe, arxiv:1802.07880 (2018)

Algebraic Quantum Field Theory

An Algebraic Approach to Quantum Field Theory, R. Haag, D. Kastler, Journal of Mathematical Physics, 5 (7), (1964)
Having established that certain physical systems are Markov random fields, how do we use them for machine learning?

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

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

We will now implement the lattice ϕ^4 field theory/Ising model to represent interactions of agents who aim to buy or sell a stock in the context of financial markets.



Lattice ϕ^4 field theory as a multi-agent system of financial markets, D. Bachtis, arxiv:2411.15813.

D. Bachtis, D. Berman, in preparation.

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We want to model two interactions:

1) People tend to imitate the behaviour of their neighbours

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We want to model two interactions:

- 1) People tend to imitate the behaviour of their neighbours
- 2) People are influenced by the opinion of the majority or the minority

Our model will then represent two types of agents

1) Fundamentalists, agents who invest based on the fundamental value of an asset. For example, a fundamentalist might decide to buy an asset when it is undervalued or sell an asset when it resides above the fundamental value.

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- 1) Fundamentalists, agents who invest based on the fundamental value of an asset. For example, a fundamentalist might decide to buy an asset when it is undervalued or sell an asset when it resides above the fundamental value.
- 2) Chartists or noise traders, agents who invest based on emerging trends (i.e. by relying on "charts") rather than the fundamental value of an asset. A chartist who is invested in an undervalued asset might decide to spontaneously sell the asset due to a momentary and emerging trend.

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This information already exists in the Hamiltonian of the Ising model or the lattice action of the ϕ^4 theory due to the Z₂ symmetry breaking phase transition!

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This information already exists in the Hamiltonian of the Ising model or the lattice action of the ϕ^4 theory due to the Z₂ symmetry breaking phase transition!

$$H = -J \sum_{\langle ij \rangle} s_i s_j$$
$$S = -\sum_{\langle ij \rangle} \phi_i \phi_j + \left(d + \frac{\mu^2}{2}\right) \sum_i \phi_i^2 + \frac{\lambda}{4} \sum_i \phi_i^4$$

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- 2) People are influenced by the opinion of the majority or the minority
- This information does not exist in the Hamiltonian or lattice action and we need to explicitly introduce it.
- We observe that the intensive magnetization, i.e. the sum over all the degrees of freedom in the lattice, represents the opinion of the majority.
- We can then introduce a term in the Hamiltonian that forces an agent to take into consideration the opinion of the majority or minority via the magnetization.

$$-s_i \left| \frac{1}{N} \sum_{j,j \in \Lambda} s_j \right|$$

The physical behaviour that we obtain from the multi-agent ϕ^4 model of financial markets:



The ϕ^4 multi-agent model can reproduce nontrivial aspects of financial markets, called stylized facts, such as volatility clustering and fat-tailed probability distribution of returns.





To employ quantum field-theoretic or statistical mechanical algorithms for other machine learning tasks, we need to define a form of asymmetric distance between two probability distributions, called the Kullback-Leibler divergence:

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

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

Α _____ Β

1.

We can use the first definition of the Kullback-Leibler divergence:

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

to minimize the asymmetric distance between our model probability distribution p and an <u>unknown</u> empirical probability distribution q for <u>which we have data available</u>.

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We can use the second definition of the Kullback-Leibler divergence:

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

to minimize the asymmetric distance between our model probability distribution p and a <u>known</u> empirical probability distribution q for <u>which we do not have data available</u>.

Let's first investigate the case of a <u>known</u> empirical probability distribution q for <u>which we do</u> <u>not have data available</u>.

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

We want to minimize the Kullback-Leibler divergence.

We consider that $q(\phi)$ is the probability distribution of a system described by a new Hamiltonian or action A.

By minimizing the KL divergence we will make the two probability distributions equal. We can then use the probability distribution $p(\varphi; \theta)$ of the φ^4 theory to draw samples from the target distribution $q(\varphi)$.

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

Gibbs-Bogoliubov-Feynman Inequality

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

<> denotes expectation value

There are two important observations on the above equation:

- 1. It sets a rigorous upper bound to the calculation of the free energy of the system with action A.
- 2. The bound is dependent entirely on samples drawn from the distribution $p(\phi;\theta)$ of the ϕ^4 theory.

As a very simple proof-of-principle demonstration, we can consider a disordered lattice action of the ϕ^4 theory:

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

that is able to represent more intricate actions, such as actions that include longer range interactions



What if the target probability distribution $q(\phi)$ is unknown?

We can use the first definition of the Kullback-Leibler divergence:

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

to minimize the asymmetric distance between our model probability distribution p and an <u>unknown</u> empirical probability distribution q for <u>which we have data available</u>.

We consider as an example a problem of image segmentation:



We are searching for the optimal values of the coupling constants in the ϕ^4 action that are able to reproduce the data as configurations in the equilibrium distribution.

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



So far we have investigated the behaviour of a

 ϕ^4 Markov random field



We are now interested in investigating the behaviour of a

 ϕ^4 neural network



Hidden layer

Visible layer

ϕ^4 neural network



Hidden layer Visible layer

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

The Boltzmann probability distribution of the ϕ^4 neural network is now a joint probability distribution of the visible ϕ and the hidden h variables:

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

1. Collaboration for a second seco

From the joint probability distribution of the ϕ^4 neural network

$$p(\phi, h; \theta) = rac{\exp[-S(\phi, h; \theta)]}{\int_{\phi, h} \exp[-S(\phi, h; \theta)] d\phi dh}.$$

We are able to marginalize out variables and derive marginal probability distributions $p(\phi;\theta)$ and $p(h;\theta)$:

Finden layer

$$\begin{array}{c} & & & \\ \hline h_1 & & h_2 \\ \hline \phi_1 & & \phi_2 \\ \hline \phi_1 & & \phi_2 \\ \hline \phi_1 & & \phi_n \\ \hline \end{array} \\ & & & p(\phi;\theta) = \int_{\mathbf{h}} p(\phi,\mathbf{h};\theta) d\mathbf{h} = \frac{\int_{\mathbf{h}} \exp[-S(\phi,\mathbf{h};\theta)] d\phi}{\int_{\phi,\mathbf{h}} \exp[-S(\phi,\mathbf{h};\theta)] d\phi} d\mathbf{h}, \\ & & \\ \end{array}$$
Visible layer

We now want to minimize the asymmetric distance between the empirical probability distribution $q(\phi)$ and the marginal probability distribution $p(\phi;\theta)$:

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



In other words, we want to reproduce the dataset in the visible layer. The hidden layer will then uncover dependencies on the data.

Hidden layer



Visible layer







The ϕ^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:



ϕ^4 equivalence with the Ising model (under an appropriate limit)

Quantum field-theoretic machine learning, D. Bachtis, G. Aarts and B. Lucini, Phys. Rev. D 103, 074510, (arXiv:2102.09449).

Are there "genuine" phase transitions in the learning process of neural networks?

Cascade of phase transitions in the training of energy-based models ,D. Bachtis, G. Biroli, A. Decelle, B. Seoane, Advances in Neural Information Processing Systems 37 (NeurIPS 2024).

We saw that an order parameter is a quantity which can be used to distinguish between two phases of a system. For example in the case of the Ising model, the order parameter was the magnetization.



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We consider again the case of the Bernoulli-Bernoulli restricted Boltzmann machine:

$$H = -\sum_{i,j} w_{ij} u_i h_j - \sum_i a_i u_i - \sum_j b_j h_j$$

And for simplicity we assume that $\alpha_1 = b_j = 0$, and that the visible and hidden variables take values of {-1,1}

Hidden layer



Visible layer

To study mathematically the behaviour of the restricted Boltzmann machine:

- 1) We consider that important information about the learning process of a neural network is evidently encoded within the weight matrix. We are going to extract this information via a singular value decomposition.
- 2) We rely on the implementation of techniques from statistical mechanics, such as the replica method to infer the phase diagram of the neural network and, equivalently, extract information about the order parameters which characterize the phases of the system.

Thermodynamics of Restricted Boltzmann Machines and related learning dynamics, A. Decelle, G. Fissore, C. Furtlehner, J Stat Phys 172, 1576–1608 (2018).


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α						
_	1	_	3 -	5 —	7 —	9
	2	_	4 —	6 —	8 —	10

epochs

Cascade of phase transitions in the training of energy-based models ,D. Bachtis, G. Biroli, A. Decelle, B. Seoane, Advances in Neural Information Processing Systems 37 (NeurIPS 2024).

If a phase transition is "genuine" it should persist also to the thermodynamic limit

To investigate the scaling of the phase transitions one can progressively rescale the dataset:







Numerical data are consistent with a mean-field universality class

Phase transitions might help us understand how machine learning algorithms function, but can we extract any other useful information from them?

Additional useful information about the learning process relates to the emergence of a critical slowing down effect:



A long-term ambition of studying phase transitions of neural networks is a potential quest for unification of machine learning algorithms based on universality classes:

Ising universality class:

Ising model, critical opalescence, liquid to gas phase transition, and many more...

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Ising universality class:

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Can we simplify the study of machine learning algorithms through universality?

Summary:

• Disorder

What are the connections between machine learning and disordered systems?

Prototypical types of disorder/inhomogeneity, Ising model, Ising spin glass, Ising random field, the ϕ^4 spin glass, replica theory and the overlap order parameter, intuitive connections with machine learning.

• Quantum field-theoretic (and statistical-mechanical) machine learning How can we unify statistical mechanics, quantum field theory, and machine learning under a common mathematical framework?

The (local) Markov property, Hammersley-Clifford theorem, Nelson construction of quantum field theories, ϕ^4 Markov fields, ϕ^4 multi-agent systems, reinforcement learning, ϕ^4 neural networks and their generalization of the Bernoulli-Bernoulli restricted Boltzmann machine [see Nobel Prize 2024 (Hinton)], applications.

• Phase transitions of machine learning algorithms

Are there ***genuine*** phase transitions in neural networks?

Second-order phase transitions during the learning process of neural networks, order parameters, scaling and universality in probabilistic machine learning, a quest for unification of machine learning under universality classes, numerical examples.

Thank you for your attention!