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Statistical Physics of Learning and Inference

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Abstract. The exchange of ideas between statistical physics and computer science has been very fruitful and is currently gaining momentum as a consequence of the revived interest in neural networks, machine learning and inference in general.

Statistical physics methods complement other approaches to the theoretical understanding of machine learning processes and inference in stochastic modeling. They facilitate, for instance, the study of dynamical and equilibrium properties of randomized training processes in model situations. At the same time, the approach inspires novel and efficient algorithms and facilitates interdisciplinary applications in a variety of scientific and technical disciplines.

1 Introduction

The regained popularity of machine learning in general and neural networks in particular [1–3] can be associated with at least two major trends: On the one hand, the ever-increasing amount of training data acquired in various domains facilitates the training of very powerful systems, *deep* neural networks being only the most prominent example [4–6]. On the other hand, the computational power needed for the data driven adaptation and optimization of such systems has become available quite broadly.

Both developments have made it possible to realize and deploy in practice several concepts that had been devised previously - some of them even decades ago, see [4–6] for examples and further references. In addition, and equally importantly, efficient computational techniques have been put forward, such as the use of pre-trained networks or sophisticated regularization techniques like drop-out or similar schemes [4–7]. Moreover, important modifications and conceptual extensions of the systems in use have contributed to the achieved progress significantly. With respect to the example of deep networks, this concerns, for instance, weight sharing in convolutional neural networks or the use of specific activation functions [4–6, 8].

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Recently, several authors have argued that the level of theoretical understanding does not yet parallel the impressive practical success of machine learning techniques and that many heuristic and pragmatic concepts are not understood to a satisfactory degree, see for instance [9–13] in the context of deep learning.

While the partial lack of a solid theoretical background does not belittle the practical importance and success of the methods, it is certainly worthwhile to strengthen their theoretical foundations. Obviously, the optimization of existing tools and the development of novel concepts would benefit greatly from a deeper understanding of relevant phenomena for the design and training of adaptive systems. This concerns, for instance, their mathematical and statistical foundations, the dynamics of training dynamics and convergence behavior or the expected generalization ability.

2 Statistical physics and learning

Statistical mechanics based methods have been applied in several areas outside the traditional realms of physics. For instance, analytical and computational techniques from the statistical physics of disordered sytems have been applied in various areas of computer science and statistics, including inference, machine learning and optimization.

The wide-spread availability of powerful computational resources has facilitated the diffusion of these, often very involved, methods into neighboring fields. A superb example is the efficient use of Markov Chain Monte Carlo methods, which were developed to attack problems in Statistical mechanics in the middle of the last century [14]. Analytical methods, developed for the analysis of *disordered systems* with many degrees of freedom, constitute another important example [15]. They have been applied in a variety of problems on the basis of mathematical analogies, which appear to be purely formal, at a glance.

In fact it was such an analogy, pointed out by J. Hopfield [16], which triggered considerable interest in neural networks and similar systems within the physics community, originally: the conceptual similarity of simple models for dynamical neural networks and models of disordered magnetic materials [15]. Initially equilibrium and dynamical effects in so-called attractor neural networks such as the Little-Hopfield model had been addressed [17]. Later it was realized that the same or very similar theoretical concepts can be applied to analyse the weight space of neural networks. Inspired by the groundbreaking work of E. Grander [18, 19], a large variety of machine learning scenarios have been investigated, including the supervised training of feedforward neural networks and the unsupervised analysis of structured data sets, see [20–23] for reviews. In turn, the study of machine learning processes also triggered the development and better understanding of statistical physics tools and theories.

3 Current research questions and concrete problems

This special session brings together researchers who develop or apply statistical physics related methods in the context of machine learning, data analysis and inference.

The aim is to re-establish and intensify the fruitful interaction between statistical physics related research and the machine learning community. The organizers are convinced that statistical physics based approaches will be instrumental in obtaining the urgently needed insights for the design and further improvement of efficient machine learning techniques and algorithms.

Obviously, the special session and this tutorial paper can only address a small subset of the many challenges and research topics which are relevant in this area. Tools and concepts applied in this broad context cover a wide range of concepts and areas: information theory, the mathematical analysis of stochastic differential equations, the statistical mechanics of disordered systems, the theory of phase transitions, mean field theory, Monte Carlo simulations, variational calculus, renormalization group and a variety of other analytical and computational methods [7, 15, 24–27, 27–29].

Specific topics and questions of current interest include, but are by far not limited to the following list. Where available, we provide references to tutorial papers of relevant special sessions at recent ESANN conferences.

- The relation of statistical mechanics to information theoretical methods and other approaches to computational learning theory [25, 30]

  Information processing and statistical information theory are widely used in machine learning concepts. In particular the Boltzmann-Gibbs statistics is an essential tool in adaptive processes [25, 31–33]. The measuring of mutual information and the comparison of data in terms of divergences based on respective entropy concepts stimulated new approches in machine learning data analysis [34, 35]. For example, Tsallis entropy, known from non-extensive statistical physics [36,37], can be used to improve learning in decision trees [38] and kernel based learning [39]. Recent approaches relate the Tsallis entropy also to reinforcement and causal imitation learning [40, 41].

- Learning in deep layered networks and other complex architectures [42]

  Many tools and analytical methods have been developed and applied successfully to the analysis of relatively simple, mostly shallow neural networks [7, 20–22]. Currently, their application and significant conceptual extension is gaining momentum (pun intended) in the context of deep learning and other learning paradigms, see [7, 24, 43–47] for recent examples of these on-going efforts.

- Emergent behavior in societies of interacting agents

  Simple models of societies have been used to show that some social science problems are, at least in principle, not outside the reach of mathematical modeling, see [48, 49] for examples and further references. To go beyond the analysis of simple two-state agents it seems reasonable to add more ingredients in the agent's model. These could include learning from the interaction with other agents and the capability of analyzing issues that can only be represented in multidimensional spaces. The modeling of societies of neural networks presents the type of problem that can be dealt with the methods and ideas of statistical mechanics.

- Symmetry breaking and transient dynamics in training processes
  Symmetry breaking phase transitions in neural networks and other learning systems have been a topic of great interest, see [7, 20–22, 51–53] for many examples and references. Their counterpart in off-equilibrium online learning scenarios are quasi-stationary plateau states in the learning curves [23, 50, 54–56]. The existence of these plateaux is in general a sign of symmetries that can often be only broken after the computational effort of including more data. Methods to analyse, identify, and possibly to partially alleviate these problems in simple feedforward networks have been presented in the context of statistical mechanics, see [50, 54–56] for some of the many examples. The problem of saddle-point plateau states has recently re-gained attention within the deep learning community, see e.g. [44].

- Equilibrium phenomena in vector quantization

  Phase transitions and equilibrium phenomena were intensively studied also in the context of self-organizing maps for unsupervised vector quantization and topographic vector quantization [57, 58]. Particularly, phase transitions in the context of violations of topology preservation in self-organizing maps (SOM) in dependence on the range of interacting neurons in the neural lattices were investigated applying Fokker- Planck-approaches [59, 60]. Moreover, energy function for those networks were considered in [61, 62] and [63]. Ordering processes and asymptotic behavior of SOMs were studied in terms of stationary states in particle systems of interacting particles delivering results for [61, 64, 65].

- Theoretical approaches to consciousness

  No agreement on what consciousness is seems to be around the corner [66]. However, some measures of casual relationships in complex systems, see e.g. [67], have been put forward as possible ways to discuss how to recognize when a certain degree of consciousness can be attributed to a system. Integrated information has been presented in several forms, including versions of Tononi's information integration [68, 69] based on information theory. Since the current state of the theory permits dealing with very few degrees of freedom, methods from the repertoire developed to study neural networks as versions of disordered systems, are a real possibility for advance our understanding in this field.

Without going into detail, we only mention some of the further topics of interest and on-going research:

- Design and anlysis of interpretable models and *white-box* systems [70–72]
- Probabilistic inference in stochastic systems and complex networks
- Learning in model space
- Transfer learning and lifelong learning in non-stationary environments [73]
- Complex optimization problems and related algorithmic approaches.

The diversity of methodological approaches inspired by statistical physics leads to a plethora of potential applications. The relevant scientific disciplines and application areas include neurosciences, systems biology and bioinformatics, environmental modelling, social sciences and signal processing, to name just very few examples. Methods borrowed from statistical physics continue to play an important role in the development all of these challenging areas.

4 Contributions to the ESANN 2019 special session on the "Statistical physics of learning and inference"

The three accepted contributions to the special session address a selection of diverse topics, which reflect the relevance of statistical physics ideas and concepts in a variety of areas.

Trust law and ideology in a NN agent model of the US Appellate Courts
In their contribution [74], N. Caticha and F. Alves employ systems of interacting neural networks as mathematica models of judicial panels. The authors investigate the the role of ideological bias, dampening and amplification effects in the decision process.

Noise helps optimization escape from saddle points in the neural dynamics
Synaptic plasticity is in the focus of a contribution by Y. Fang, Z. Yu and F. Chen [75]. The authors investigate the influence of saddle points and the role of noise in learning processes. Mathematical analysis and computer experiments demonstrate how noise can improve the performance of optimization strategies in this context.

On-line learning dynamics of ReLU neural networks using statistical physics techniques
The statistical physics of on-line learning is revisited in a contribution by M. Straat and M. Biehl [76]. They study the training of layered neural networks with rectified linear units (ReLU) from a stream of example data. Emphasis is put on the role of the specific activation function for the occurrance of sub-optimal quasi-stationary plateau states in the learning dynamics.

Statistical physics has contributed significantly to the investigation and understanding of relevant phenomena in machine learning and inference, and it continues to do so. We hope that the contributions to this special session on the "Statistical physics of learning and inference" helps to increase attention among active machine learning researchers.

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