Décima Escuela de Física-Matemática

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Machine Learning for Quantum Matter and Technology

Departamento de Matemáticas – Departamento de Física

Universidad de los Andes

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Posters

Morning Lectures

Statistical mechanics and Monte Carlo simulations

Monte Carlo methods are considered one of the largest and most important class of numerical methods used for solving statistical mechanics problems. We will offer a brief overview of the statistical mechanics followed by an introduction to Monte Carlo methods in the context of statistical physics and quantum mechanics. The material covers the simulation of equilibrium systems and the theoretical basis of important Monte Carlo algorithms and ideas such as the Metropolis algorithm in detail. We will devote the part of the afternoons to the computer implementation, exploration, and application of these ideas through coding examples.

Introduction to elements of machine learning

We will introduce foundational ideas and models in machine learning ranging from concepts like supervised and unsupervised learning, to linear and logistic regression, multilayer perceptrons, convolutional neural networks, recurrent neural networks, optimization strategies, overfitting, generalization, regularization, as well as demonstrate how these models can be applied to problems in a variety of simple physical scenarios in statistical and many-body physics. We will dedicate part of the afternoons to practice exercises that will give you hands-on experience implementing these ideas and algorithms on datasets generated from statistical physics models. These exercises will teach you how to implement machine learning algorithms with TensorFlow and other open source libraries used in modern deep learning research.

Generative models, ML-inspired representations of quantum state, and applications in quantum physics and technology

Unsupervised learning, in particular generative models, have been recently shown to have the potential to solve problems in quantum physics and quantum technology. We will introduce energy-based generative models as well as modern generative models used in state-of-the-art machine learning research and will focus on application and extensions of these ideas in areas such as quantum state tomography, energy minimization of variational wave functions, and quantum error correction. We will dedicate part of the afternoons to practice exercises that will give you hands-on experience implementing energy minimization (using NetKet) and quantum state tomography with neural networks using and QuCumber, a specialized software developed at the Perimeter Institute Quantum Intelligence Lab for quantum state reconstruction using ML ideas.

Short Communications

Andrés Ángel
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Universidad de Los Andes, Bogotá, Colombia

Some examples of topological data analysis

Topological data analysis is a recent area that tries to quantify the shape of data. I will present two of the main tools to represent the topological nature of data. The Mapper graph and Persistence diagrams. I will present simple examples using R packages.

John Goodrick
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Intrinsic complexity of algorithmic learning: a logical and combinatorial perspective

In 1984, Valiant introduced the notion of "Probably Approximately Correct" (PAC) learnability of a concept class (a set C of possible "hypotheses" predicting labelings of instances). Roughly, a concept class C is PAC learnable if there is some learning algorithm which is guaranteed to ("probably and approximately") learn a true hypothesis from C if it is given enough training samples, independently of the distribution according to which they are selected. Surprisingly, whether or not a class is PAC learnable is equivalent to a purely combinatorial condition on the complexity of C, namely that C should have finite Vapnik-Chervonenkis dimension, and is also equivalent to the existence of certain kinds of compression schemes for encoding lists of training instances (by the proof in 2015 of "Warmuth's Conjecture" by Moran and Yehudayoff). The concept of VC-dimension, in turn, has been extensively studied by researchers in mathematical logic, which has supplied rich families of new PAC-learnable classes.

We will summarize these interesting connections between machine learning, combinatorics, and logic, and discuss recent advances by Hunter Chase and James Freitag on links between various notions of algorithmic learning (online learning, equivalence query learning) and other combinatorial complexity functions.

Reference: "Model theory and machine learning," Chase and Freitag,
https://arxiv.org/abs/1801.06566.

Andreas Griewank
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High dimensional integration of kinks and jumps - Smoothing by preintegration

We show how simple kinks and jumps of otherwise smooth integrands over $\mathbb{R}^d$ can be dealt with by a preliminary integration with respect to a single well chosen variable. It is assumed that this preintegration, or conditional sampling, can be carried out with negligible error, which is the case in particular for option pricing problems. It is proven that under appropriate conditions the preintegrated function of $d-1$ variables belongs to appropriate mixed Sobolev spaces, so potentially allowing high efficiency of Quasi Monte Carlo and Sparse Grid Methods applied to the preintegrated problem. The efficiency of applying Quasi Monte Carlo to the preintegrated function are demonstrated on a digital Asian option using the Principal Component Analysis factorization of the covariance matrix.

Joint work with Frances Y. Kuo, Hernan Leövey, Ian H. Sloan.

Adolfo Alejandro Hernández Cásares
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Localization and Artificial Gauge Fields in Quantum Optical Lattices

Ultracold neutral atoms in optical lattices can be used for quantum simulation of Lattice Gauge Theories specially those involving U(1) which correspond to magnetic fields. In this case we focus on a 2D lattice with an extra particle or extra hole (with an extra phase on quantum hoping term due to Aharonov-Bohm effect) finding interesting features as the Hofstadter's Butterfly spectrum, particle-hole symmetries and a new localization effect equivalent to that predicted by the Lorentz force if the particles had positive or negative charge, suggesting the presence of a synthetic magnetic force acting on both particles and holes.

Héctor Iván Reyes
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Machine Learning for Spectrum Sensing. Our experiments.

In this speech, I will talk about the application of machine learning methods to spectrum sensing. Spectrum sensing is a task performed by communications equipment for determining the occupancy of radiofrequency channels. Detecting unocuppied channels allows transmitters to discover spectrum holes to be used opportunistically. We conducted experiments with GNU Radio, an open source software for implementing radios, to test different machine learning methods. In this talk we propose three GNU Radio blocks for performing spectrum sensing based on the autocorrelation of samples captured with an SDR device such as HackRF One, RTL-SDR or USRP. The proposed blocks analyze the autocorrelation of samples through different methods to determine if they come from either noise or signals transmitted by communication devices. The reason for using the autocorrelation is that this feature is different for noise and for communication signals regardless of the noise power, which is an advantage in comparison with energy detection, another common method for spectrum sensing, which requires knowledge of the noise level to determine the presence or absence of communication signals. The first method consists in calculating the Euclidean distance between the autocorrelation and a reference line defined by the maximum values taken by the autocorrelation with high signal to noise ratio samples. To perform spectrum sensing with this method the proposed block takes the samples, calculates the autocorrelation and its distance to the reference line; if the distance is above certain threshold the block decides that the samples are signal, otherwise that the samples are noise. The second method consists in clustering the points defined by the variance and the mean of the autocorrelation samples. For implementing this method we identify one cluster containing samples with only noise, and other clusters containing samples from different communication signals. To put into practice this method, the block takes samples and estimates to which cluster they belong. The third method is based on the percentiles (25%, 50%, 75%) of the autocorrelation fast Fourier transform, better known as the power spectral density (PSD). For this method, we calculate the percentiles of the PSD of noise and communication signals at different frequencies and labeled them accordingly. We use the percentiles and their corresponding labels to train a KNN (K-nearest neighbor) classifier and create a classification model. To apply this method the proposed block takes the received samples, calculates the percentiles of their PSD and feeds them to the KNN model, which decides whether the samples come from either noise or communication signals. We implemented and tested experimentally the aforementioned methods with GNU radio companion, HackRF one, and RTL-SDR 2832u. In the talk we will present details about the proposed methods, their performance evaluation and the experiments conducted during the process.

Julián Rincón
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Understanding continuous quantum matter via matrix product states

The first half of the talk will introduce matrix product states as an ansatz that can efficiently describe weakly-entangled wave functions of quantum many-body local Hamiltonians. I will review their formulation both in the discrete for lattice models, and in the continuum for quantum field theories. The second part of the talk will focus on a quasi-exact algorithm that accurately finds the ground state of non-relativistic 1+1 dimensional quantum field theories. Using this algorithm, I will describe the ground state properties of a Lieb-Liniger-like model with exponentially decaying interactions.

Ángel Rojas
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A Target Oriented Averaging Search Trajectory and its Application to Artificial Neural Network Training

Artificial Neural Network Training (ANNT) usually involves nonsmooth objective functions to be minimized. This optimization problem is currently solved by randomized local methods in order to handle the nonsmoothness and to improve the chance of reaching a global minimizer. Usually, the training methods depends on the direction of steepest descent such as Gradient Descent (GD) or Stochastic Gradient Descent (SGD) for not getting stuck at stationary points [BCN18]. Further [ACGH18] proves convergence of GD to a low local minimizer in the weights space under certain strong assumptions on the smooth objective and a random initialization scheme. Though, in practice, these statistical learning algorithms work quite well using backpropagation, we develop a deterministic global optimization algorithm called SALGO which employs a **T**arget **O**riented **A**veraging **S**earch **T**rajectory namely TOAST. Actually, the label describes that the search direction is an average of the steepest descent direction combined linearly by the initial point of search and proportional to certain sensitivity determined by a target level of search [Gri81]. The analalog of SALGO is the Gradient Momentum Method but differs of its stochastic versions [LR17]. Also, the sensitivity and the target level are two method parameters which are selected by the user or set by suitable heuristics to reach a low minimizer of the ANN's empirical risk. Typically, the reachable level in machine learning is positive and rather close to zero, so the target level can be set accordingly and reduce it until a tolerance. A main difference between our approach and backpropagation is that the latter

disregards the nonsmoothness of the empirical risk. In contrast, we handle the "nondifferentiabilites" of the empirical risk surface through its Succesive Abs-Linearization proposed in [Gri13],[GWS],[GW18]. Finally, we focus on ANN depending on hinge functions (a.k.a ReLU) as the activation function of the hidden states. Its implementation is due to the results in [ZBH+16] and allows us to formulate explicitly our TOAST formula when the sensitivity $e = 1$. We proved this ANN setup guarantees that the associated empirical risk's minima are nondifferentiable. We experiment with different models where ANN and hinge functions are often used and compare them with ANN trained by SGD and GD.

Joint work with Andreas Griewank.

Palabras Clave: Successive Piecewise Linearization, Quadratic Regularization, Abs-Normal Form, Generalized descent

References

[ACGH18] Sanjeev Arora, Nadav Cohen, Noah Golowich, and Wei Hu. A convergence analysis of gradient descent for deep linear neural networks. *arXiv preprint arXiv:1810.02281*, 2018.

[BCN18] Léon Bottou, Frank E Curtis, and Jorge Nocedal. Optimization methods for large-scale machine learning. *Siam Review*, 60(2):223–311, 2018.

[Gri81] Andreas O Griewank. Generalized descent for global optimization. *Journal of optimization theory and applications*, 34(1):11–39, 1981.

[Gri13] Andreas Griewank. On stable piecewise linearization and generalized algorithmic differentiation. *Optimization Methods and Software*, 28(6):1139–1178, 2013.

[GW18] Andreas Griewank and Andrea Walther. Finite convergence of an active signature method to local minima of piecewise linear functions. *Optimization Methods and Software*, pages 1–21, 2018.

[GWS] Andreas Griewank, Andrea Walther, and Preprint Number SPP1962. Priority programme 1962.

[LR17] Nicolas Loizou and Peter Richtárik. Momentum and stochastic momentum for stochastic gradient, newton, proximal point and subspace descent methods. *arXiv preprint arXiv:1712.09677*, 2017.

[ZBH+16] Chiyuan Zhang, Samy Bengio, Moritz Hardt, Benjamin Recht, and Oriol Vinyals. Understanding deep learning requires rethinking generalization. *arXiv preprint arXiv:1611.03530*, 2016.

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Distribuciones de Máxima Entropía en Bolas de Wasserstein

Presentamos un método para hallar la distribución de máxima entropía en la Bola de Wasserstein de un radio dado t centrada en la distribución empírica dada por n puntos. Esta distribución es la más general (minimiza la cantidad de información previa) a una distancia t de la distribución empírica y de aquí su importancia en inferencia estadística. El método depende de un nuevo algoritmo de cutting plane y es generalizado a otro tipo de funciones, entre ellas los Funcionales Euclidianos Subaditivos. También, damos una nueva generalización al algoritmo de Fortune para generar el diagrama de Voronoi Pesado Aditivamente que permite hacer optimización en Bolas de Wasserstein a mayor velocidad.

Mauricio Velasco
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Learning on graphs and the Wasserstein nuclear norm

In this talk we will focus on the problem of detecting "communities" on graphs. Our main contribution is that this and other machine learning problems on graphs can be reformulated as instances of robust optimization problems with the appropriate Wasserstein norm. We will prove new theoretical guarantees for community discovery in the stochastic block model and introduce new ADMM algorithms for practically solving these problems on relatively large graphs extending work of Esfahani-Kuhn and Recht-Fazel-Parrilo. These results are joint work with Daniel De Roux. (Note: The talk will be self-contained and will not assume previous knowledge of robust optimization.)

Joint work with Daniel De Roux..

Posters

Leonel Ardila, Juan Flórez
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Continuous Normalizing Flows applied to RBM

Among the generative models in machine learning one is of particular interest for the physicists, this model is the Restricted Boltzmann Machine (RBM). A great work has been done on both it's inner working and how to efficiently train it [Fis14], however there are a lot of open questions regarding this model. We focus on the training of and RBM and propose a new way to train it based on the recent results regarding Continuous Normalizing Flows [CRBD18] and previous work on the application of Gibbs Flows to generate arbitrary distributions [JH15]. The scheme proposed is tested on RBM's with both Gaussian visible units and uniformly distributed visible units, and a approach to train Deep Belief Networks is presented. The continuous normalizing flow formalism allows to know the probability of a given state of the neural network, hence, it gives a much more reliable framework to train generative models, and can be helpful to numerically estimate the value of the partition function for energy based generative models; to estimate the value of the partition function is a useful tool to numerically test results on how the training of an RBM is related to it's free energy [Dom17].

References

[CRBD18] R. T. Q. Chen, Y. Rubanova, J. Bettencourt, and D. Duvenaud. Neural ordinary differential equations. *NIPS 2018 Proceedings*, 2018.

[Dom17] S. Domingos. Nonequilibrium thermodynamics of restricted botlzmann machines. *Physical Review E*, 96, 2017.

[Fis14] A. Fischer. *Training restricted Boltzmann machines.* Tesis de doctorado, Faculty of science, University of Copenhagen, Copenhagen, Dinamarca, 2014.

[JH15] Y. Pokern J. Heng, A. Doucet. Gibbs flow for approximate transport with applications to bayesian computation. *arXiv preprint arXiv:1509.0878*, 2015.

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Machine Learning flux visualization as a wing turbulence test

In the last 20 years, flux visualization has re-emerged as a quantitative technique due to the advances in digital image analysis. Despite of that, the main image analysis methods present low efficiency and poor precision. An easy and efficient way to obtain results in this topic is a Machine Learning (ML) approach. In this work, GoogLeNet(Inception v1) was retrained by mean of Schlieren local images, which were obtained from systems with a known and well defined Reynolds number to test airflow passing through a wing-shaped profile, looking for local turbulence characterization when the critical angle is overpassed.

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Mutual information of a fully connected neuronal network learning process

Artificial Neural Networks (ANN) were developed in the last 50 years with the intention to mimic the brain's process to handle stimuli [Sch15]. Thanks to increasing computing power at lower costs, ANN have finally become a central feature to the success of the broader Machine Learning (ML) community. [BL09, CW08, GFDF04, GZ93, Gol16, KWR+01]. Biological studies have found that weak correlations among pairs of neurons coexist with strong correlations in the states of population as a whole. [SBSB06]. In this work we want to test whether these correlations also hold for ANN. To this end we train fully connected neuronal network (FCNN) for different classification tasks and measure the mutual information (MI) between groups of neurons at different stages of the learning process of the mentioned neural network. Our results suggest that FCNNs behave as their biological counterpart, that is, the global MI is larger than the local one by an order of magnitude. We finalize by discussing the implications of these results for ANN training.

Joint work with J. Forero-Romero, J.M. Pedraza.

References

[BL09] Roman M. Balabin and Ekaterina I. Lomakina. Neural network approach to quantum-chemistry data: Accurate prediction of density functional theory energies. *The Journal of Chemical Physics*, 131(7):074104, August 2009.

[CW08] Ronan Collobert and Jason Weston. A Unified Architecture for Natural Language Processing: Deep Neural Networks with Multitask Learning. In *Proceedings of the 25th International Conference on Machine Learning*, ICML '08, pages 160–167, New York, NY, USA, 2008. ACM. event-place: Helsinki, Finland.

[GFDF04] Ernest V. Garcia, Tracy L. Faber, Cooke C. David, and Russell D. Folks. Computer Analysis of Nuclear Cardiology Procedures. In *Emission Tomography*, pages 541–550. Elsevier, 2004.

[Gol16] Yoav Goldberg. A Primer on Neural Network Models for Natural Language Processing. *Journal of Artificial Intelligence Research*, 57:345–420, November 2016.

[GZ93] Johann Gasteiger and Jure Zupan. Neural Networks in Chemistry. *Angewandte Chemie International Edition in English*, 32(4):503–527, 1993.

[KWR+01] Javed Khan, Jun S. Wei, Markus Ringnér, Lao H. Saal, Marc Ladanyi, Frank Westermann, Frank Berthold, Manfred Schwab, Cristina R. Antonescu, Carsten Peterson, and Paul S. Meltzer. Classification and diagnostic prediction of cancers using gene expression profiling and artificial neural networks. *Nature Medicine*, 7(6):673–679, June 2001.

[SBSB06] Elad Schneidman, Michael J. Berry, Ronen Segev, and William Bialek. Weak pairwise correlations imply strongly correlated network states in a neural population. *Nature*, 440(7087):1007–1012, April 2006.

[Sch15] Jürgen Schmidhuber. Deep learning in neural networks: An overview. *Neural Networks*, 61:85–117, January 2015.

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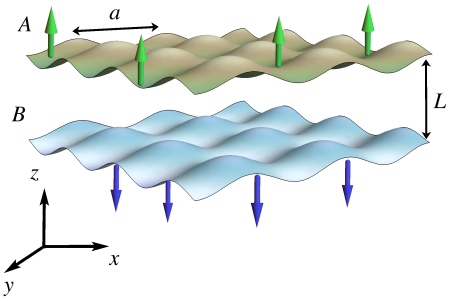
p-wave Superfluid Phases of Fermi Molecules in a Bilayer Lattice Array

We investigate the emergence of superfluid $p_x + ip_y$ phases in an ultracold gas of dipolar molecules lying in two parallel square lattices in 2D. Also, we determine two zero temperature phase diagrams of this Fermi system, both of them exhibit stable $p-$wave superfluid phases as well as a phase separation region as a function of the dipole-dipole interaction coupling. Finally, we estimate the Berezinskii-Kosterlitz-Thouless critical temperature of the superfluid in the lattice and discuss possible experimental realizations. $p-$wave superfluid phases may lead to possible applications in quantum information and quantum computations.



Schematic representation of dipolar Fermi molecules situated in a bilayer array composed of parallel optical lattices in two dimensions
Joint work with R. Paredes.

Alejandro Ferrero Botero
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Universidad Catlólica de Colombia, Bogotá, Colombia.

Solution to Green Functions Using the Finite Difference Method

Green functions have a great importance in mathematics and physics to solve differential equations with given boundary conditions. This presentation shows how the Finite Difference method can be used to solve Green functions with Dirichlet, Neumann, or mixed boundary conditions. It is indicated how to programm the code in *python*.
Since most of the physical systems can be modeled by means of second order differential equations, this work is focused on solving ordinary differential equations of the form $\mathcal{L}\{G(x,x')\} = \delta(x-x')$, where $\mathcal{L}$ is an arbitrary second order differential operator.
It is also explained how the Green function can be used to solve some physical systems of great importance such as the driven damped harmonic oscillator, electrostatic potentials with some symmetries, among others.

Solución a funciones de Green Mediante el Método de Diferenicas Finitas

Las funciones de Green son de gran importancia en el área de la física y las matemáticas para resolver ecuaciones diferenciales con condiciones de frontera dadas. En esta presentación se muestra cómo el método de diferencias finitas puede ser usado para resolver funciones de Green con condiciones de frontera de Dirichlet, Neumann, o combinación de éstas. Se indica como hacer la programación en el lenguaje *python*.
Dado que la gran mayoría de sistemas físicos pueden ser modelados mediante ecuaciones diferenciales de segundo grado, este trabajo se enfoca en resolver ecuaciones diferenciales ordinarias de la forma $\mathcal{L}\{G(x,x')\} = \delta(x-x')$, donde $\mathcal{L}$ es un operador diferencial de segundo grado arbitrario.

Se explica, además, como la función de Green encontrada se puede utilizar para resolver varios sistemas físicos de gran importancia como el oscilador armónico forzado y amortiguado, potenciales electrostáticos con ciertas simetrías presentes, entre otros.

Santiago Figueroa Manrique
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Towards a quantum Monte Carlo for lattice systems

In this work we build the foundations of a quantum Monte Carlo (QMC) as a numerical method to solve lattice many-body quantum systems with nearest-neighbor interactions. As motivation, we briefly describe a system of repulsively interacting spin-1 bosons in an optical lattice at unit filling in the Mott insulator phase with an external quadratic Zeeman field. QMC methods circumvent the difficulties that arise on these type of systems by mapping the quantum partition function into the one of an effective classical model and then, implementing a Monte Carlo sampling of the new partition function. Such a mapping is performed by the means of the Suzuki-Trotter decomposition, which transforms the original partition function into a summation of world lines. Finally, we show how the Metropolis algorithm can be implemented to sample the world lines, thus allowing us to measure certain type of observables.

Víctor Alfonso Loaiza Moreno
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Universidad del Valle, Cali, Colombia.

A quantum treatment of the anisotropic diamagnetic Kepler problem in a silicon crystal with low concentration of phosphorus impurities

In this work we study the anisotropic diamagnetic Kepler problem which is related with the behavior of electron interaction with low densities of phosphorus impurities in a silicon crystal focusing on the case of a magnetic field along the [111] direction of the crystal. Here we propose a full quantum description to this problem by choosing an appropriate basis and implementing the complex rotation method to study the resonance states. Within this approach we were able to reproduce and improve reported results on the bound spectrum of the field free and the diamagnetic anisotropic Kepler problem. Furthermore, we report here for the first time an spectrum above the first Landau ionization threshold.

Mateo Londoño
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Optimización de un esquema de control multi-paso para la estabilización vibracional de moléculas diatómicas

En las últimas dos décadas se han dedicado esfuerzos considerables, tanto experimentales como teóricos, a la formación de moléculas frías y ultrafrías, debido a su importancia para la comprensión del comportamiento de la materia a temperaturas cercanas al cero absoluto. En la estrategia de fotoasosiación, se usan pulsos láser para estabilizar vibracionalmente en el estado electrónico fundamental las moléculas, a partir de colisiones binarias en gases a $T < 1$mK. Para el diseño de pulsos óptimos, la teoría del control óptimo cuántico (QOC) ha resultado útil. en particular, se han propuesto esquemas basados en métodos de optimización heurísticos basados en algoritmos genéticos. En este trabajo se implementa computacionalmente un esquema de tres pulsos para la estabilización vibracional en el estado basal de singulete de una molécula de KRb, la cual se encuentra inicialmente atrapada en una resonancioa de Feschbach del primer estado triplete. En el primer paso, se implemeta un esquema ladder descending en el infrarrojo para llevar el diátomo a un nivel de baja energa del primer estado triplete. En el segundo y tercer pasos, se implementa un esquema pump-dump para llevar el diátomo a un segundo estado triplete, el cual se encuntra acoplado con un estado singulete excitado, y desde allí hacia el nivel basal del estado singulete fundamental. Encontramos que nuestra estrategia es mucho más eficiente que estrategias que solo consideran pulsos pump-dump.

Joint work with Julio C. Arce.

Fernando Naranjo Mayorga, Nicanor Poveda Tejada, Oscar Fabián Téquita Vargas.
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Neuronal Electronic Synchronization Between the Model Morris-Lecar and the RCLSJ Circuit

The RCSLJ model (resistance, capacitance, inductance, Josephson junction) can simulate neuronal electrical activity. The article presents a description of how this circuit can simulate the behavior of neuronal discharges of the biological model Morris-Lecar (M-L). The problem is presented in the synchronization of the model M-L with the circuit, for this, we introduce an adaptive control scheme using Lyapunov functions to analytically calculate a controlling function that allows us the synchronization. The results confirm that the controller, with appropriate gain coefficients, makes generalized synchronization (identical frequencies but not amplitudes) and full synchronization (frequencies and identical amplitudes) between the circuit and the M-L model effective. With the results, we can control the dynamic behavior of the RCLSJ system to reproduce the neuronal electrical behavior of the Morris-Lecar model. The synchronization of these models could show a path towards the understanding of neuronal electrical activity.

Palabras Clave: Josephson junctions, RCLSJ circuit, Lyapunov functions, model Morris-Lecar, control- ling function.

Jairo José Orozco Sandoval
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Discovering Phase transitions using unsupervised machine learning PCA

Machine learning, specific subset of artificial intelligence, trains a machine to learn from unexplored data. It has become a robust method for the identification of patterns within complex physical systems to determine certain physical quantities without prior knowledge of their physics principles. For many years classifying and discovering phases and phase transitions is one of the most important topics in Condensed Matter Physics; however, it is not an easy job to do, especially when we work with complex systems and the number of states is very large. In this work we applied unsupervised machine learning called Principal Component Analysis (PCA) to square and hexagonal Ising model to identify phases and phase transitions. We found that PCA allow us to identify these phase transitions and located the critical points for both systems. We demonstrated that the firsts principal components are related with physical properties of the model as the order parameter and the

susceptibility. The weight vectors in PCA have a physical explanation, which is helpful to get a better understanding of the system's behavior. The critical temperature T_c in square and hexagonal systems were determined. For the square system a $T_c = 2.26339 J/K_B$ was obtained and for the hexagonal system a $T_c = 1.51508 J/K_B$, having a 0.5% percent error from the true thermodynamic critical temperature.

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The SSH model in the momentum representation

This work is based on the Su-Schrieffer-Heeger model, which describes a system of non-interacting polarized fermions, i.e. without spin, moving in a one-dimensional superlattice. We analyze the Hamiltonian of the system in second quantization, in which the optical lattice has discretized the space, and take into account that the basis that diagonalizes the kinetic energy is the one of momentum. In the first case, let us consider a finite chain; we show that the discrete Sine transform type-I respects the finite boundary conditions of the system, hence, it is the proper transform to be used. This transformation arises from linear combinations of plane waves and allows us to express our Hamiltonian in the momentum basis in such a way that will allow us to extend the study of the system to an arbitrary number of sites. In the second case, when periodic boundary conditions are considered, the usual Fourier transform can be used; this case will be shortly discussed in this poster as well.

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Feature Extraction of Neural Networks Applied to Magnetic Models

This undergraduate thesis studies the weight matrices of a neural network trained and evaluated in spin samples, in order to identify which physical quantities the network uses to solve the magnetic phase classification problem. A Densely Connected Neural Network was coded in order to classify the phases of the square-lattice Ising model. Several hidden layers sizes were tested in order to determine an optimal model, which was then analysed using Principal Component Analysis and K-means clustering. This analysis separated the weight matrices in three distinct classes, two of them specialising in positive and negative magnetisation and a third one that activates in both cases. It was also found that these

weight matrices reflected the translational invariance and Ising symmetry of the model. Finally, a possible implementation of the same method on the one dimensional quantum XY-model is proposed.

References

[AOT18] S. Arai, M. Ohzeki, and K. Tanaka. Deep Neural Network Detects Quantum Phase Transition. *Journal of the Physical Society of Japan*, 87(3):033001, March 2018. arXiv: 1712.00371.

[Bea18] Matthew J. S. Beach. Machine learning vortices at the Kosterlitz-Thouless transition. *Physical Review B*, 97(4), 2018.

[CL00] P. M. Chaikin and T. C. Lubensky. *Principles of Condensed Matter Physics*. Cambridge University Press, Cambridge, October 2000.

[CM17] J Carrasquilla and R. G. Melko. Machine learning phases of matter. *Nature Physics*, 13(5):431–434, February 2017. arXiv: 1605.01735.

[Coo98] A. C. C. Coolen. *A Beginner's Guide to the Mathematics of Neural Networks*. Springer, 1998.

[DD96] G. Deco and Obradovic D. *An Information-Theoretic Approach to Neural Computing (Perspectives in Neural Computing)*. Springer, 1st edition, 1996.

[Gom18] D. Gomez. Physics monograph on Ising Model analysis based on KPCA: tarod13/Monograph, September 2018. original-date: 2018-08-16T16:14:42Z.

[Hay09] S. O. Haykin. *Neural Networks and Learning Machines, Simon O. Haykin*. Pearson Education, 6th edition, 2009.

[JWHT13] G. James, D. Witten, T. Hastie, and R. Tibshirani. *An Introduction to Statistical Learning: with Applications in R*. Springer-Verlag New York Inc., New York, 1st ed. 2013, corr. 7th printing 2017 edition, June 2013.

[KSH12] A. Krizhevsky, I. Sutskever, and G. E. Hinton. ImageNet Classification with Deep Convolutional Neural Networks. In F. Pereira, C. J. C. Burges, L. Bottou, and K. Q. Weinberger, editors, *Advances in Neural Information Processing Systems 25*, pages 1097–1105. Curran Associates, Inc., 2012.

[KYW13] D. Kuzum, S. Yu, and H.-S. Philip Wong. Synaptic electronics: materials, devices and applications. *Nanotechnology*, 24(38):382001, 2013.

[Mac03] D. J. C Mackay. Information Theory, Inference and Learning Algorithms: David J. C. MacKay, 2003.

[Oha] V. Ohanyan. Introduction to Quantum Spin Chains Lecture Notes, (56 hours).

[Por] J. Portilla. Complete Guide to TensorFlow for Deep Learning with Python.

[Qua09] H. T. Quan. Finite-Temperature Scaling of Magnetic Susceptibility and Geometric Phase in the XY Spin Chain. *Journal of Physics A: Mathematical and Theoretical*, 42(39):395002, October 2009. arXiv: 0806.2476.

[RD17] L Ridderstolpe and G. Dibitetto. Exact Solutions of the Ising Model, 2017. https://uu.diva-portal.org/smash/get/diva2:1139470/FULLTEXT01.pdf.

[Sto14] G. Stolz. Introduction to the Mathematics of the XY -Spin Chain, 2014.

[SW18] P. Suchsland and S. Wessel. Parameter diagnostics of phases and phase transition learning by neural networks. *Physical Review B*, February 2018.

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Reconstructing the Universe with Machine Learning.

Machine learning has found its way into observational cosmology by tackling on of the most relevant problems in the field: infering the large scale distribution of Dark Matter (DM) in the local Universe. The DM spatial distribution is not directly observable and must be inferred from the observational data. In this talk we will show how machine learning methods can help us to solve this task. As training data-sets we use different two kinds of cosmological simulations: hydrodynamical and semi-analytic. We will present preliminary results for our reconstruction efforts based on SDSS data and comment on its implications and strategies for improvement.

Joint work with J. Forero-Romero.

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Assisted Optimal Transfer of Excitonic Energy by Deep Reinforcement Learning

Light-matter interaction in light-harvesting systems is a hottest topic in molecular physics. Due to its numerous applications in quantum and photovoltaic systems, understanding its performance is of paramount relevance in improving efficiency of the current devices. This research proposes the application of reinforcement learning with neural networks like

alternative to uncover the design principles behind efficiency and application to other fields such as dynamical systems and control theory.

Joint work with Leonardo A. Pachón.

References

[FTWM18] Thomas Fösel, Petru Tighineanu, Talitha Weiss, and Florian Marquardt. Reinforcement learning with neural networks for quantum feedback. *Physical Review X*, 8(3):031084, 2018.

[MBW+19] Pankaj Mehta, Marin Bukov, Ching-Hao Wang, Alexandre GR Day, Clint Richardson, Charles K Fisher, and David J Schwab. A high-bias, low-variance introduction to machine learning for physicists. *Physics Reports*, 2019.

[PBB17] Leonardo A Pachón, Juan D Botero, and Paul Brumer. Open system perspective on incoherent excitation of light-harvesting systems. *Journal of Physics B: Atomic, Molecular and Optical Physics*, 50(18):184003, 2017.

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Neural Networks as Variational Wavefunctions

The use of deep learning algorithms for solving quantum mechanics problems is a relatively new, interdisciplinary field of study. Recent approaches include the identification of phases and phase transitions on condensed-matter Hamiltonians using feedforward neural networks [CM17]; the use of a restricted Boltzmann machine for dimensionality reduction of the ground state many-body wavefunction [CT17, CNI18]; the use of a perceptron as a variational anszats for finding the ground state of typical Hamiltonian systems [Ten18] and the use of deep learning for molecular generation and optimization of quantum materials for photovoltaic applications [EBFC19]. The main goal of this work is to implement current state-of-the-art algorithms that use neural networks as generic variational anszats, in order to test them on systems of higher complexity, and potentially find alternative neural network architectures that can compete with the aforementioned methods. We have currently reproduced the results reported in [Ten18] using an unsupervised neural network architecture that allows the training of more than one hidden layer, and we have, as ongoing work, performed the implementation of the computational method proposed in [CT17] for solving extended quantum many-body systems beyond those treated in [CT17].

Joint work with Javier Madroñero, John Henry Reina.

References

[CM17] Juan Carrasquilla and Roger G. Melko. Machine learning phases of matter. *Nature Physics*, 13:431 EP –, Feb 2017.

[CNI18] Giuseppe Carleo, Yusuke Nomura, and Masatoshi Imada. Constructing exact representations of quantum many-body systems with deep neural networks. *Nature Communications*, 9(1):5322, 2018.

[CT17] Giuseppe Carleo and Matthias Troyer. Solving the quantum many-body problem with artificial neural networks. *Science*, 355(6325):602–606, 2017.

[EBFC19] Daniel C. Elton, Zois Boukouvalas, Mark D. Fuge, and Peter W. Chung. Deep learning for molecular generation and optimization - a review of the state of the art. *CoRR*, abs/1903.04388, 2019.

[Ten18] Peiyuan Teng. Machine-learning quantum mechanics: Solving quantum mechanics problems using radial basis function networks. *Phys. Rev. E*, 98:033305, Sep 2018.

Monday, May 27th (Room: W-101, W-102, W-404)

8:00 – 9:00	*Registration*
9:00 – 9:15	*Opening*
9:15 – 10:15	Roger Melko: *Introduction to Many-Body physics*
10:15 – 11:15	Roger Melko: *Introduction to Monte Carlo simulations*
11:15 – 11:45	Break
11:45 – 12:45	Roger Melko: *Monte Carlo Tutorial in Python*
12:45 – 14:00	Lunch Break
14:00 – 15:00	Practical Session (Estelle Inack)
15:00 – 15:30	Break
15:30 – 16:10	Julián Rincón: *Understanding continuous quantum matter via matrix product states*
16:10 – 16:50	Héctor Reyes: *Machine Learning for Spectrum Sensing. Our experiments.*

Tuesday, May 28th (Room: W-102, ML-607, ML-615)	
9:00 – 10:00	Juan Carrasquilla: *Introduction to machine learning*
10:00 – 11:00	Juan Carrasquilla: *Neural networks and backpropagation*
11:00 – 11:30	Break
11:30 – 12:30	Estelle Inack: *Feed-forward neural networks and Tensorflow (Room ML-606, ML-607, ML-615)*
12:30 – 14:00	Lunch Break
Room W-101, ML-606, ML-615	
14:00 – 14:25	Ángel Rojas: *A Target Oriented Averaging Search Trajectory and its Application to Artificial Neural Network Training*
14:25 – 14:50	Adolfo Hernández: *Localization and Artificial Gauge Fields in Quantum Optical Lattices*
14:50 – 15:15	Luis Felipe Vargas: *Distribuciones de Máxima Entropía en Bolas de Wasserstein*
15:15 – 15:40	Break
15:40 – 16:40	Practical Session (Estelle Inack)
16:40 – 17:00	Break
17:00 –	Poster Session & refreshments

Wednesday, May 29th (Room: W-101, ML-607, ML-615)	
9:00 – 10:00	Juan Carrasquilla: *Unsupervised learning, maximum likelihood, PCA, t-SNE*
10:00 – 11:00	Giacomo Torlai: *Restricted Boltzmann machines (RBM) I.*
11:00 – 11:30	Break
11:30 – 12:30	Estelle Inack: *Unsupervised learning tutorial: PCA, t-SNE*

Thursday, May 30th (Room: B-202, C-104)

9:00 – 10:00	Giacomo Torlai: *Restricted Boltzmann machines (RBM) II.*
10:00 – 11:00	Giacomo Torlai: *Quantum state reconstruction*
11:00 – 11:30	Break
11:30 – 12:30	Estelle Inack: *Learning thermal states with RBMs tutorial*
12:30 – 14:00	Lunch Break
14:00 – 14:40	John Goodrick: *Intrinsic complexity of algorithmic learning: a logical and combinatorial perspective*
14:40 – 15:20	Andrés Ángel: *Some examples of topological data analysis*
15:20 – 15:50	Break
15:50 – 16:50	Practical Session (Estelle Inack)

Friday, May 31st (Room: B-202, C-104)

9:00 – 10:00	Estelle Inack: *Variational Monte Carlo*
10:00 – 11:00	Estelle Inack: *VMC Tutorial*
11:00 – 11:30	Break
11:30 – 12:30	Practical Session (Estelle Inack)
12:30 – 14:00	Lunch Break
14:00 – 15:00	Practical Session (Estelle Inack)
15:00 – 15:30	Break
15:30 – 16:10	Andreas Griewank: *High dimensional integration of kinks and jumps - Smoothing by preintegration*
16:10 – 16:50	Mauricio Velasco: *Learning on graphs and the Wasserstein nuclear norm*
17:00 –	Entrega de certificados de asistencia

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	Monday	Tuesday	Wednesday	Thursday	Friday
8:00 – 9:00	Registration				
9:00 – 10:00	R. Melko	J. Carrasquilla	J. Carrasquilla	G. Torlai	E. Inack
10:00 – 11:00	R. Melko	J. Carrasquilla	G. Torlai	G. Torlai	E. Inack
11:00 – 11:30	*Break*	*Break*	*Break*	*Break*	*Break*
11:30 – 12:30	R. Melko	E. Inack	E. Inack	E. Inack	E. Inack
12:30 – 14:00	*Break*	*Break*		*Break*	*Break*
	14:00 – 15:00 Problem Session	14:00 – 14:25 A. Rojas		14:00 – 14:40 J. Goodrick T	14:00 – 15:00 Problem Session
	15:00 – 15:30 *Break*	14:25–14:50 A. Hernández		14:40-15:20 A. Ángel	15:00 – 15:30 *Break*
	15:30-16:10 J. Rincón	14:50–15:15 A. Hernández		15:20 – 15:50 *Break*	15:30-16:10 A. Griewank
	16:10-16:50 H. Reyes	15:15 – 15:40 *Break*		15:20 – 15:50 Problem Session	16:10–16:50 M. Velasco
		15:40 – 16:40 Problem Session			17:00 Entrega de certificados
		16:40–17:00 *Break*			
		17:00 Poster Session			