Franco Nori: Machine Learning Applied to Computationally Difficult Problems in Quantum Physics: Full Summit Transcript

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Machine Learning Applied to Computationally Difficult Problems in Quantum Physics

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My name is Franco Nori. Is a great pleasure to be here and I thank you for attending this meeting, and I'll be talking about some of the work we are doing within the NTT PHI group. I would like to thank the organizers for putting together this very interesting event. The topics studied by NTT PHI are very exciting, and I'm glad to be part of this great team. Let me first start with a brief overview of just a few interactions between our team and other groups within NTT PHI. After this brief overview of these interactions, then I'm going to start talking about machine learning and neural networks applied to computationally difficult problems in quantum physics.

The first one I would like to raise is the following. Is it possible to have decoherence-free interaction between qubits? And the proposed solution was a postdoc and a visitor and myself some years ago was to study decoherence-free interaction between giant atoms made of superconducting qubits in the context of waveguide quantum electrodynamics.

The theoretical prediction was confirmed by a very nice experiment performed by Will Oliver's group at MIT was published a few months ago in Nature, and it's called "Waveguide quantum electrodynamics with superconducting artificial giant atoms." And this is the first joint MIT Michigan Nature paper during this NTT PHI grant period. And we're very pleased with this. And I look forward to having additional collaborations like this one also, with other NTT PHI groups. Another collaboration inside NTT PHI regards the “Quantum Hall effects in a rapidly rotating polariton condensate.” And this work is mainly driven by two people, Michael Fraser and Yoshihisa Yamamoto.

They are the main driving forces of this project and this has been a great fun. We’re also interacting inside the NTT PHI environment with the groups of Marandi at Caltech, McMahon at Cornell, Oliver at MIT, and as I mentioned before, Fraser-Yamamoto at NTT, and others at NTT PHI are also very welcome to interact with us. NTT PHI is interested in various topics, including how to use neural networks to solve computationally difficult and important problems. Let us now look at one example of using neural networks to study computationally difficult and hard problems.

Everything we’ll be talking today is mostly work in progress to be extended and improved in the future. So the first example I would like to discuss is topological quantum phase transition retrieved through manifold learning, which is a variety of version of machine learning. This work is done in collaboration with Che, Gneiting and Liu all members of the group, preprint is available in the Arxiv. Some groups are studying a quantum-enhanced machine learning where machine learning is supposed to be used in actual quantum computers to use exponential speed-up and using quantum error correction; we’re not working on these kind of things we’re doing something different.

We’re studying how to apply machine learning, applied to quantum problems. For example, how to identify quantum phases and phase transitions. We shall be talking about right now. How to achieve, how to perform quantum state tomography in a more efficient manner. That’s another work of ours, which I’ll be showing later on. And how to assist the experimental data analysis which is a separate project, which we recently published. But I will not discuss today because the experiments can produce massive amounts of data and machine learning can help to understand this huge tsunami of data provided by these experiments.

Machine learning can be either supervised or unsupervised. Supervised requires human-labeled data. So we have here the blue dots have a label. The red dots have a different label. And the question is the new data corresponds to either the blue category or the red category. And many of these problems in machine learning they use the example of identifying cats and dogs, but this is typical example. However, there are the cases which are also provides with there are no labels. So you’re looking at the cluster structure, and you need to define a metric, a distance between the different points to be able to correlate them together to create these clusters. And manifold learning is ideally suited to look at problems we just did on non-linearities and unsupervised.

Using the principal component analysis along this green axis here which are the principal axis here, you can actually identify a simple structure with linear projection when you increase the axis here, you get the red dots in one area, and the blue dots down here. But, in general, you could get red green, yellow, blue dots in a complicated manner and the correlations are better seen when you do an nonlinear embedding. And in unsupervised learning the colors represent similarities, are not labels because there are no prior labels here.

So we are interested in using machine learning to identify topological quantum phases. And this requires looking at the actual phases and their boundaries. And you start from a set of Hamiltonians or wave functions. And recall that this is difficult to do because there is no symmetry breaking, there is no local order parameters and in complicated cases you cannot compute the topological properties analytically, and numerically is very hard. So, therefore, machine learning is enriching the toolbox for studying topological quantum phase transitions. And before our work, there were quite a few groups looking at supervised machine learning. The shortcomings that you need to have prior knowledge of the system and the data must be labeled for each phase.

This is needed in order to train the neural network. More recently in the past few years, there has been increased push on looking at unsupervised and nonlinear embeddings. One of the shortcomings we have seen is that they all use the Euclidean distance which is a natural way to construct the similarity matrix. But we have proven that it is suboptimal. It is not the optimal way to look at distance. The Chebyshev distances provides better performance. So, therefore, the difficulty here is how to detect topological quantum phase transition is a challenge because there is no local order parameters.

Few years ago, we thought well, three or so years ago, machine learning may provide effective methods for identifying topological features. And in the past few years, the past two years several groups are moving this direction. And we have shown that one type of machine learning called manifold learning can successfully retrieve topological quantum phase transitions in momentum and real spaces. We have also shown that if you use the Chebyshev distance between data points as supposed to Euclidean distance, you sharpen the characteristic features of these topological quantum phases in momentum space, and then afterwards we do so-called diffusion map, isometric map can be applied to implement the dimensionality reduction and to learn about these phases and phase transition in an unsupervised manner.

So this is a summary of this work on how to characterize and study topological phases. And the example we used is to look at the canonical famous models like the SSH model, the QWZ model, the quenched SSH model. We look at this momentum space and the real space, and we found that the method works very well in all of these models. And moreover provides implications and demonstrations for learning also in real space where the topological invariants could be either unknown or hard to compute. So it provides insight on both momentum space and real space, and the capability of manifold learning is very good especially when you have the suitable metric in exploring topological quantum phase transition.

So this is one area we would like to keep working on, topological phases and how to detect them. Of course, there are other problems where neural networks can be useful to solve computationally hard and important problems in quantum physics. And one of them is quantum state tomography, which is important to evaluate the quality of state production experiments. The problem is quantum state tomography scales really bad. It is impossible to perform it for six and a half, or 20 qubits. If you have 2,000 or more forget it, it’s not going to work.

So now we’re seeing a very important process, which is one here tomography, which cannot be done because there is a computationally hard bottleneck. So machine learning is designed to efficiently handle big data. So the question we’re asking a few years ago is can machine learning help us to solve this bottleneck, which is quantum state tomography. And this is a project called Eigenstate extraction with neural-network tomography, with a student [Abhijeeet] Melkani, research scientist of the group Clemens Gneiting, and I’ll be brief in summarizing this now. The specific machine learning paradigm is the standard artificial neural networks. They have been recently shown in the past couple of years to be successful for tomography of pure states. Our approach will be to carry this over to mixed states. And this is done by successively reconstructing the eigenstates or the mixed states. So it is an iterative procedure, where you can slowly, slowly get into the desired target state. If you wish to see more details, this has been recently published in Phys Rev A and has been selected as an editor suggestion, which means like some of the referees liked it.

So tomography is very hard to do, but it's important and machine learning can help us to do that using neural networks, and this to achieve mixed-state tomography using an iterative eigenstate reconstruction. So why it is so challenging? Because you're trying to reconstruct the quantum states from measurements. You have a single qubit, you have a few Pauli matrices, essentially there are very few measurements to make. When you have N qubits then the N appears in the exponent. So the number of measurements grows exponentially, and this exponential scaling makes the computation to be very difficult. It's prohibitively expensive for large system sizes. So this is the bottleneck, is these exponential dependence on the number of qubits. So by the time you get to 20 or 24 it is impossible. It gets even worse. Experimental data is noisy and therefore you need to consider maximum-likelihood estimation in order to reconstruct the quantum state that kind of fits the measurements best.

And, again, these are expensive. There was a seminal work some time ago on ion traps. The post-processing for eight qubits took them an entire week. There were different ideas proposed regarding compressed sensing to reduce measurements, linear regression, et cetera. But they all have problems and you quickly hit a wall. There's no way to avoid it. Indeed, the initial estimate is that to do tomography for 14 qubits state, you will take centuries, and you cannot support a graduate student for a century because you need to pay your retirement benefits and it is simply complicated. So, therefore, a team here sometime ago, we're looking at the question of how to do a full reconstruction of 14-qubit state within four hours.

Actually, it was three point three hours, though sometime ago. And many experimental groups were telling us that was very popular paper to read and study because they wanted to do fast quantum state tomography. They could not support the student for one or two centuries. They wanted to get the results quickly. And then because we need to get these density matrices and then they need to do these measurements here. But when you have n qubits the number of expectation values go like four to the n, so the Pauli matrices becomes much bigger. A maximum likelihood makes it even more time consuming. And this is the paper by the group in Innsbruck, where they go this one-week post-processing and there were speed-ups done by different groups and hours. Also how to do 14 qubit tomography in four hours, using linear regression. But the next question is can machine learning help with quantum state tomography? Can allow us to give us the tools to do the next step to improve it even further.

And then the standard one is this one here. Therefore, for neural networks there are some inputs here, X1, X2, X3. There are some weighting factors when you get an output function phi we just call nonlinear activation function that could be heavy side Signum, piecewise, linear, logistic, hyperbolic. And this creates a decision boundary and input space where you get let's say the red one, the red dots on the left and the blue dots on the right. Some separation between them. And you could have either two layers or three layers or n number of layers, can do either shallow or deep. This can allow you to approximate any continuous function. You can train data via some cost function minimization. And then there are different varieties of neural nets. We're looking at some sequel-restricted Boltzmann machine. Restricted means that the input layer spins are not talking to each other. The output layers spins are not talking to each other. And we got reasonably good results with the input layer, output layer, no hidden layer, and the probability of finding a spin configuration goes like the Boltzmann factor.

So we try to leverage pure-state tomography for mixed-state tomography. By doing an iterative process where you start here. So there are the mixed states in the blue area, the pure states boundary here. And then the initial state is here with the iterative process you get closer and closer to the actual mixed state. And then eventually once you get here, you do the final jump inside. So you're looking at a dominant eigenstate which is closest pure state and then compute some measurements and then do an iterative algorithm that to make you approach this desired state. And after you do that then you can essentially compare results with some data. We got some data for four to eight trapped-ion qubits approximate W states were produced and they were looking at let's say the dominant eigenstate is reliably recorded for any equal four, five six, seven, eight for the eigenstate, for the eigenvalues we're still working because we're getting some resolution or not as accurate as we would like to, so this is still work in progress, but for the States is working really well.

So there is some cost scaling, which is beneficial, goes like n as opposed to n squared. And then the most relevant information on the quality of the state production is retrieved directly. This works for flexible rank. And so it is possible to extract the eigenstate within network tomography. It is cost-effective and scalable and delivers the most relevant information about state generation. And it's an interesting and viable use case for machine learning in quantum physics. We're also now more recently working on how to do quantum state tomography using Conditional Generative Adversarial Networks.

[Unintelligible] the masters student are analyzed in PhD and then two former postdocs. So this CGAN refers to this Conditional Generative Adversarial Networks. In this framework you have two neural networks which are essentially having a dual, they're competing with each other. And one of them is called generator, another one is called discriminator. And there they're learning multi-modal models from the data. And then we improved these by adding a cost of neural network layers that enable the conversion of outputs from any standard neural network into physical density matrix.

So, therefore, to reconstruct the density matrix, the generator layer and the discriminator networks, so the two networks, they must train each other on data using standard gradient-based methods. So, we demonstrate that our quantum state tomography and the adversarial network can reconstruct the optical quantum state with very high fidelity, which is orders of magnitude faster and from less data than a standard maximum likelihood method. So we're excited about this. We also show that this quantum state tomography with these adversarial networks can reconstruct a quantum state in a single evolution of the generator network, if it has been pre-trained on similar quantum states. So requires some additional training. And all of these is still work in progress where some preliminary results written up but we're continuing. And I would like to thank all of you for attending this talk. And thanks again for the invitation.