QTML 2020 POSTER INFORMATION

Poster Session #1 Overview

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Poster Session 1

November 11, 9:00-10:30am EST

#1	**Modeling and Control of a Reconfigurable Photonic Circuit using Deep Learning** Robert Chapman, Akram Youssry, Alberto Peruzzo, Christopher Ferrie and Marco Tomamichel

As reconfigurable quantum photonic circuits grow in complexity, they become increasingly challenging to model and control. Not only can the structure of the internal Hamiltonian be unknown, but also the electrical control signals can suffer from drift and coupling losses can distort the optical measurement. Here, we present a deep neural network to model and control a programmable photonic continuous-time quantum walk. We develop a novel "grey-box" approach where we treat unknown parameters, such as the form of the Hamiltonian and the electrical control response as a "black-box", while treating the known components, including Hamiltonian evolution and measurements analytically as a "white-box". We demonstrate high-performance on a simulator of the chip for modelling and subsequently preparing desired unitaries, with typical fidelities >99%. Our method is efficient in the number of required parameters and fully generic to the quantum circuit design and physical hardware.

#2	**Variational Quantum Boltzmann Machines** Christa Zoufal, Aurelien Lucchi and Stefan Woerner

This work presents a novel realization approach to Quantum Boltzmann Machines (QBMs). The preparation of the required Gibbs states, as well as the evaluation of the loss function's analytic gradient, is based on Variational Quantum Imaginary Time Evolution, a technique that is typically used for ground state computation. In contrast to existing methods, this implementation facilitates near-term compatible QBM training with gradients of the actual loss function for arbitrary parameterized Hamiltonians which do not necessarily have to be fully-visible but may also include hidden units. The variational Gibbs state approximation is demonstrated with numerical simulations and experiments run on real quantum hardware provided by IBM Quantum. Furthermore, we illustrate the application of this variational QBM approach to generative and discriminative learning tasks using numerical simulation.

#3	**Variational quantum Gibbs state preparation with a truncated Taylor series** Youle Wang, Guangxi Li and Xin Wang

The preparation of quantum Gibbs state is an essential part of quantum computation and has wide-ranging applications in various areas, including quantum simulation, quantum optimization, and quantum machine learning. In this paper, we propose variational hybrid quantum-classical algorithms for quantum Gibbs state preparation. We first utilize a truncated Taylor series to evaluate the free energy and choose the truncated free energy as the loss function. Our protocol then trains the parameterized quantum circuits to learn the desired quantum Gibbs state. Notably, this algorithm can be implemented on near-term quantum computers equipped with parameterized quantum circuits. By performing numerical experiments, we show that shallow parameterized circuits with only one additional qubit can be trained to prepare the Ising chain and spin chain Gibbs states with a fidelity higher than 95%. In particular, for the Ising chain model, we find that a simplified circuit ansatz with only one parameter and one additional qubit can be trained to realize a 99% fidelity in Gibbs state preparation at inverse temperatures larger than 2.

#4	**A variational toolbox for quantum multi-parameter estimation** Johannes Jakob Meyer, Johannes Borregaard and Jens Eisert

With an ever-expanding ecosystem of noisy and intermediate-scale quantum devices, exploring their possible applications is a rapidly growing field of quantum information science. In this work, we demonstrate that variational quantum algorithms feasible on such devices address a challenge central to the field of quantum metrology: The identification of near-optimal probes and measurement operators for noisy multi-parameter estimation problems. We first introduce a general framework which allows for sequential updates of variational parameters to improve probe states and measurements and is widely applicable to both discrete and continuous variable settings. We then demonstrate the practical functioning of the approach through numerical simulations, showcasing how tailored probes and measurements improve over standard methods in the noisy regime. Along the way, we prove the validity of a general parameter-shift rule for noisy evolutions, expected to be of general interest in variational quantum algorithms. In our approach, we advocate the mindset of quantum-aided design, exploiting quantum technology to learn close to optimal, experimentally feasible quantum metrology protocols.

#5	**A Quantum Approach to the Minimum Dominating Set Problem** Jaeho Choi, Seunghyeok Oh, Seunghoon Park and Joongheon Kim

In recent years, there are interests in hybrid quantum-classical algorithms related to the AI field increasing rapidly. In particular, the application researches on the Quantum Approximate Optimization Algorithm (QAOA), a well-known hybrid quantum-classical algorithm suitable for solving problems based on graphs, are being conducted in various ways. Our research proposes a quantum approach using QAOA to solve the Minimum Dominating Set (MDS) problem used for limited resource allocation. In more detail, this research constructs the Hamiltonians which correspond to the constraints and the objectives on the MDS problem and transform it to be applicable to QAOA sequences. To show the novelty of the proposed approach, the simulations are performed with proper parameter learning on the actual graphs, i.e., various random 3-regular graphs. The simulation results verify the adequacy of Hamiltonian modeling for the MDS problem. This research results also prove that the hybrid quantum-classical algorithm can be applied to many real-world problems.

#6	**Integrating Machine Learning into Quantum Physics** Mogens Dalgaard

Quantum based technologies have huge potential to revolutionize various different areas such as sensing, communication, simulation, and computation. Realizing these technologies requires, among other things, improvements in our ability to control the underlying quantum systems. Quantum Optimal Control Theory attempts to face this challenge from the theoretical side. Here optimization methods that relies on gradient-based search have successfully been developed and applied within the field. However, not all quantum control tasks are suitable for gradient-based search methods. These include discrete optimization problems, or problems with noise or filtering effects where the gradient becomes too expensive to calculate. In addition, gradient- or Hessian-based searches tend to get stuck at local optima, whereas global search strategies may be more efficient.
In our work, we utilized AlphaZero to take on three different quantum control problems for unitary gate synthesis on a Circuit QED system. We used the same algorithmic hyperparameters for each problem.

The three problems consisted of a discrete control case (where gradient-based search is not applicable), a control problem that included modelling filtering effects (where gradient-based search is inefficient), and a control problem with piecewise constant pulses (where gradient-based search is highly efficient). For each problem, we benchmarked AlphaZero against conventional optimization methods typically applied within the field. For the two first problems, AlphaZero clearly outperformed the other methods leading to huge improvements in gate fidelities. However, for the last problem, gradient-based search was actually better. This motivated us to develop a Hybrid algorithm that combined AlphaZero with gradient-based search, and this hybrid algorithm outperformed both AlphaZero and gradient-based search. This hybrid algorithm thus represents a step towards integrating Machine Learning methods into Quantum Control and Engineering.
In a somewhat different vein, our group is also involved in exploring how gamified interfaces can allow novices and experts to use their experience and insights to solve quantum problems. In the Alice Challenge, participants remotely controlled a cold-atom experiment to produce Bose-Einstein condensates (BECs). Via intelligent interface design, participants were able to achieve larger BECs than our experimental team. More recently, we have extended this work into the realm of quantum simulation. That is, we are building the Quantum Pattern Matching game, which takes simulated images from a fermionic quantum gas microscope and challenges players to classify the images based on the theoretical framework used to generate the images. With this, we hope to better understand how humans think about complex problems in physics.

#7	**Binary Classification with Classical Instances and Quantum Labels** Matthias C. Caro

In classical statistical learning theory, one of the most well studied problems is that of binary classification. The information-theoretic sample complexity of this task is tightly characterized by the Vapnik-Chervonenkis (VC) dimension (Blumer et al., 1989; Hanneke, 2016). A quantum analog of this task, with training data given as a quantum state (Bshouty and Jackson, 1998) has also been intensely studied and is now known to have the same sample complexity as its classical counterpart (Arunachalam and de Wolf, 2018).
We propose a novel quantum version of the classical binary classification task by considering maps with classical input and quantum output and corresponding classical-quantum training data. We discuss learning strategies for the agnostic and for the realizable case and study their performance to obtain sample complexity upper bounds. Moreover, we provide sample complexity lower bounds which show that our upper bounds are essentially tight for pure output states. In particular, we see that the sample complexity is the same as in the classical binary classification task w.r.t. its dependence on accuracy, confidence and the VC-dimension.

#8	**A quantum active learning algorithm for sampling against adversarial attacks** Pablo Antonio Moreno Casares and Miguel Ángel Martin-Delgado

Adversarial attacks represent a serious menace for learning algorithms and may compromise the security of future autonomous systems. A theorem by Khoury and Hadfield-Menell (KH), provides sufficient conditions to guarantee the robustness of machine learning algorithms, but comes with a caveat: it is crucial to know the smallest distance among the classes of the corresponding classification problem. We propose a theoretical framework that allows us to think of active learning as sampling the most promising new points to be classified, so that the minimum distance between classes can be found and the theorem KH used. Additionally, we introduce a quantum active learning algorithm that makes

use of such framework and whose complexity is polylogarithmic in the dimension of the space, m, and the size of the initial training data n, provided the use of qRAMs; and polynomial in the precision, achieving an exponential speedup over the equivalent classical algorithm in n and m. This algorithm may be nevertheless `dequantized' reducing the advantage to polynomial.

#9	**Predicting excited states from ground state wavefunction by supervised quantum machine learning** Hiroki Kawai and Yuya O. Nakagawa

Excited states of molecules lie in the heart of photochemistry and chemical reactions. The recent development in quantum computational chemistry leads to inventions of a variety of algorithms that calculate the excited states of molecules on near-term quantum computers, but they require more computational burdens than the algorithms for calculating the ground states. In this study, we propose a scheme of supervised quantum machine learning which predicts the excited-state properties of molecules only from their ground state wavefunction resulting in reducing the computational cost for calculating the excited states. Our model is comprised of a quantum reservoir and a classical machine learning unit which processes the measurement results of single-qubit Pauli operators with the output state from the reservoir. The quantum reservoir effectively transforms the single-qubit operators into complicated multi-qubit ones which contain essential information of the system, so that the classical machine learning unit may decode them appropriately. The number of runs for quantum computers is saved by training only the classical machine learning unit, and the whole model requires modest resources of quantum hardware that may be implemented in current experiments. We illustrate the predictive ability of our model by numerical simulations for small molecules with and without noise inevitable in near-term quantum computers. The results show that our scheme well reproduces the first and second excitation energies as well as the transition dipole moment between the ground states and excited states only from the ground state as an input. We expect our contribution will enhance the applications of quantum computers in the study of quantum chemistry and quantum materials.

#10	**Physical quantum reservoir computing for time series processing** Yudai Suzuki, Qi Gao and Naoki Yamamoto

Quantum reservoir computing is a type of machine-learning scheme that exploits the nonlinearity of a dissipative quantum dynamics for temporal information processing. In a recent study of quantum reservoir computing, an artificially-engineered reservoir is introduced to model the system, which was implemented on a noisy gate-based quantum device to test its performance. Here the artificially-engineered reservoir means that the target dissipative dynamics is realized by ensemble averaging of the system dynamics with different input states; this could lower the speed for information processing. In this study, we propose a new quantum reservoir computing scheme based on natural physical reservoir on a superconducting quantum device; this system makes full use of the realistic (un-modeled) noise that can couple neighboring qubits, which is called the crosstalk. The point of this scheme is that, thanks to the intrinsic dissipative nature, it does not need ensemble averaging, which as a result may enable a high-speed information processing. In particular we consider the system composed of multiple small reservoirs interacting with one another via crosstalk. Note that, hence, our quantum reservoir computer is hardware-specific and must be implemented on a real device. Here, we utilize the IBM superconducting quantum processors to demonstrate the performance for two tasks of sequential data

processing; an emulation of the Nonlinear AutoRegressive Moving Average dynamics (NARMA task: Fig. 1) and classification of two digit images ((5,3)-MNIST classification task: Fig. 2). For NARMA task, We observed that our quantum reservoir with 12 qubits on 'ibmq_16_melbourne' can approximate a given 100 time-steps trajectory with the normalized mean squared error (NMSE) = 2.1 × 10−6, while a simple classical linear regression can achieve (NMSE) = 7.5 × 10−4. For (5,3)-MNIST classification task, the reservoir with 28 qubits on 'ibmq_rochester' can classify 5 and 3 digit images with the training accuracies 0.85 and 0.84, respectively, which are almost the same performance achieved via the typical classical linear regression method; but the test accuracy of our reservoir is 0.73, while the linear regression achieved 0.75. A possible option for the improvement will be to utilize more qubits (small reservoir systems) to enhance the complex dynamics of the reservoir system. These results indicate that a natural physical quantum reservoir realized on a noisy quantum computer is a promising candidate for practical time series processing.

#11	**Data-based learning of predictive models with quantum memory advantage** Chengran Yang, Mile Gu, Jayne Thompson, Oscar Dahlsten, Feiyang Liu, Nora Tischler, Man-Hong Yung and Andrew Garner

Predicting a stochastic process's future statistics from past observation is a fundamental problem of many fields. Classical predictive extract information from past and replicate the future. Much of the efforts are dedicated to finding predictive models that require the least amount of past information. The ε-machines are probably optimal predictive models, which encode the past information into classical states. The entropy of these classical states is minimal among all predictive models.

Recent studies show that quantum models can go beyond the classical limit and further compress the past information. Rather than using classical states, quantum models encode past information into quantum states, which can be highly non-orthogonal and even highly linearly dependent. These features provide quantum models unbounded memory advantages over classical ε-machine. However, to-date the focus has been on exact quantum models, the limited memory available in practical scenarios might preclude their realization. This necessitates approximate models that operate with a given amount of memory. For approximate models a key metric of success is the accuracy. It has to our knowledge been an open question whether there is a quantum advantage for accuracy, when comparing quantum models to classical with the same amount of memory. A key hurdle to answer this question is to construct such quantum models.

We present a systematic method---an algorithm---for determining quantum models with encodings of optimised accuracy, given only the data of a classical stochastic process and the desired model memory dimension. Our algorithm solely uses the output data of a stochastic process. The tolerated error for the model can be set to zero, or a finite number. We demonstrate the power of our algorithm by applying it to datasets sampled from three different stochastic processes, showing numerically that the resulting quantum models successfully compress past information and accurately predict future statistics. We find through our algorithm that these quantum models can have significantly lower dimension than their zero-error counterparts. Moreover, we demonstrate examples where the approximate quantum model provably has significantly less error compared with any approximate classical model of the same dimension.

#12	**Boosting on the shoulders of giants** Alex Wozniakowski, Jayne Thompson, Mile Gu and Felix Binder

Learning from a dearth of data is among the most pressing challenges in machine learning, whereby new approaches aim to bridge the gap between efficient human learning and machine learning. As humans almost never learn new concepts in a vacuum, transferring prior domain knowledge to machine learners is paramount in the low data regime. Inspired by the process of human research, wherein scientific progress derives from prior scientific knowledge, we introduce a new approach to learning from a dearth of experimental data, which emulates the scientific paradigm of ``standing on the shoulders of giants.'' We demonstrate the efficacy of this approach in a superconducting quantum device calibration application with a limited supply of real experimental data, and we show that the machine learned concept is over 20% more accurate than the state-of-the-art. To our knowledge, our result is the first machine learned concept in the low experimental data regime, which surpasses contemporary predictive methods in physics.

#13	**Learning dynamics in many-body quantum systems** Paolo P. Mazza, Igor Lesanovsky, Georg Martius, Dominik Zietlow and Sabine Andergassen

Simulating the dynamics of a many-body interacting quantum systems is something of utmost importance for the understanding the collective quantum phenomena and for a possible future application of quantum technologies. However, this task is tremendously difficult due to the exponential growth of the Hilbert space with the systems-size. A possible tool to overcome this problem is the use of Machine Learning algorithms.
We apply ML-oriented codes for studying the dynamics of interacting quantum systems. In particular we apply a multi-layer perceptron (MLP) and a Variational AutoEncoder (VAE), to learn the time-evolution of the diagonal elements of the density matrix of the PXP model. We also try using convolutional neural networks (CNN) to see wether it is possible to learn this dynamics in a scalable way.
Knowing the evolution of the diagonal elements is of fundamental importance since they give a meaningful measure of the degree of thermalization as they do not only capture local properties but also encode spatial correlations.

#15	**Sample-efficient quantum tomography with graphical models** Abhijith Jayakumar, Marc Vuffray and Andrey Lokhov

Statistical learning theory has seen recent breakthroughs in efficient learning of undirected graphical models. It has been shown that general discrete graphical models with multi-body interactions can be learned through a convex optimization with the number of samples that achieves information-theoretical lower bound for exponential families where such bound is known. Based on these advances, we introduce a novel set of computational tools to learn graphical model representations from a few measurements of quantum many-body systems. Our method can directly incorporate symmetries of the quantum state when such prior information is available. In cases where such priors are not known, we incorporate neural nets inside our framework, acting as universal function approximators to discover a parsimonious basis representation of the energy function. The novel graphical models-based representation we introduce can also be used as variational states to minimize the energy of local Hamiltonians. Importantly, our framework is not limited to pure states and can be natively applied to any valid quantum state in full or shadow tomography settings.

#16	**Quantum Graph Neural Networks for Track Reconstruction in Particle Physics and Beyond** Cenk Tüysüz, Bilge Demirköz, Daniel Dobos, Kristiane Novotny, Karolos Potamianos, Federico Carminati, Sofia Vallecorsa, Fabio Fracas and Jean-Roch Vlimant

The Large Hadron Collider (LHC) at the European Organisation for Nuclear Research (CERN) will undergo an upgrade to further increase the instantaneous rate of particle collisions (luminosity) and become the High Luminosity LHC. This increase in luminosity, will yield many more detector hits (occupancy), and thus measurements will pose a challenge to track reconstruction algorithms being responsible to determine particle trajectories from those hits. Similar challenges exist in non-high energy physics (HEP) trajectory reconstruction use-cases. High occupancy, track density, complexity and fast growth exponentially increase the demand of algorithms in terms of time, memory and computing resources.

#17	**The theory of the quantum kernel-based binary classifier** Carsten Blank, Daniel Kyungdeock Park and Francesco Petruccione

In the NISQ era, promising quantum algorithms, in particularly in quantum machine learning, need to support a good understanding how they will perform under noise. Based on the introduction of the quantum Swap-Test classifier (2) last year at QTML 2019, we show that the STC can be “abstracted” from its implementation formulation: without index and ancilla qubit the core dynamics are described. This allows a look into the density matrix formulation, an elegant and concise form, which confirms that the similarity measure is the Hilbert-Schmidt inner product. This is significant in the situation that if information is lost due to noise – resulting in mixed states as training and/or test data undergo information destruction – the HS-inner product fails to provide a proper measure of similarity. The resulting consequences affect not only the quality of classification but also helps establishing adversarial risks during the classifier’s performance. From this observation we are making an argument to investigate density matrix formulations of common quantum machine learning algorithms. Connected to this topic, we show that a projective measurement scheme can be applied in order to calculate the probability of misclassification during a one-shot experiment. The connection to the optimal Helstrom measurement in state discrimination is seen again. Finally, we show that ensemble methods can be implemented with modifications to the initial state of the classification procedure. The models that can be trained and adjustments to the kernel itself make the STC a versatile tool.

#19	**Spin gap learning of carbenes with strongly correlated electrons** Max Schwilk, Diana N. Tahchieva and O. Anatole von Lilienfeld

Machine learning of chemical compound spaces under the presence of strongly correlated electrons is a task that has up to now hardly been addressed.
We present a carbene chemical space of eight thousand distinct compounds in which the two non-bonding molecular orbitals on a divalent carbon center are entangled in the singlet state, the QMspin data set [1].
The distinct carbene chemical characteristic of the electronic structure is monitored and singlet-triplet spin gaps are computed with higher order multireference level of theory.

Furthermore, we present accurate machine learning of the spin gaps and of the degree of orbital entanglement [2]. The strong electron correlation of the singlet state can be expressed via a multireference active space Hamiltonian. We show that characteristic electronic Coulomb and exchange interactions derived from the active space Hamiltonian can be best learned separately over the chemical space as a shortcut to detect extreme spin gap splittings and learn singlet excited states. Finally, we

show how machine learning techniques combining different levels of theory can lead to critical computational speedup and the efficient construction of approximate kernels for the learning.

#20	**Effects and mitigation of realistic readout noise in Quantum Approximate Optimization Algorithms** Filip Maciejewski, Michal Oszmaniec, Zoltán Zimborás and Flavio Baccari

Imperfect measurements contribute greatly to errors in currently available quantum devices. Recently, methods to mitigate measurement errors were proposed, relying on classical post-processing of experimental statistics, preceded by the suitable device characterization. Those techniques suffer from the curse of dimensionality due to characterization cost, sampling complexity and the complexity of post-processing, all scaling exponentially with the number of qubits. Fortunately, some interesting problems in quantum computing, including Quantum Approximate Optimization Algorithms (QAOA), require simultaneous estimation of a number of a few-particle marginals. This suggests that error mitigation techniques can be efficiently applied in this setting.

In this work we report a measurement noise model which can be efficiently described and characterized, and which admits noise-mitigation on the level of marginal probability distributions. The model can be efficiently characterized using techniques of Quantum Overlapping Tomography. We demonstrate a benchmark of the model in experiments on 11-qubits in IBM's quantum device, and conclude good agreement with theory. Finally, we analyze the effects of the proposed measurement noise model on the QAOA from two perspectives - how the noise affects the achievable optimal parameters and how it affects the final energy estimator.

#21	**Reformulation of the No-Free-Lunch Theorem for Entangled Data Sets** Kunal Sharma, Marco Cerezo, Zoe Holmes, Lukasz Cincio, Andrew Sornborger and Patrick J. Coles

The No-Free-Lunch (NFL) theorem is a celebrated result in learning theory that limits one's ability to learn a function with a training data set. With the recent rise of quantum machine learning, it is natural to ask whether there is a quantum analog of the NFL theorem, which would restrict a quantum computer's ability to learn a unitary process (the quantum analog of a function) with quantum training data. However, in the quantum setting, the training data can possess entanglement, a strong correlation with no classical analog. In this work, we show that entangled data sets lead to an apparent violation of the (classical) NFL theorem. This motivates a reformulation that accounts for the degree of entanglement in the training set. As our main result, we prove a quantum NFL theorem whereby the fundamental limit on the learnability of a unitary is reduced by entanglement. We employ Rigetti's quantum computer to test both the classical and quantum NFL theorems. Our work establishes that entanglement is a commodity in quantum machine learning.

Poster Session 2

November 11, 5:00-6:30pm EST

#1	**Online reinforcement learning of an entanglement witness** Nathan Thompson, James Steck and Elizabeth Behrman

Machine learning can be used as a systematic method to construct algorithms, that is, to non-algorithmically "program" quantum computers. Quantum machine learning enables us to perform computations without breaking down an algorithm into its gate "building blocks", eliminating that difficult step and potentially increasing efficiency by simplifying and reducing unnecessary complexity. In addition, our non-algorithmic machine learning approach is robust to both noise and to decoherence, which is ideal for running on inherently noisy NISQ devices which are limited in the number of qubits available for error correction. We demonstrate this using a fundamentally nonclassical calculation: experimentally estimating the entanglement of an unknown quantum state. Results from this have been successfully ported to the IBM hardware and the AQT trapped ion hardware simulator. We have developed and use a hybrid offline/online reinforcement learning method that includes refining training results while running on quantum hardware.

#2	**A universal hybrid quantum neural network** Ricardo Rodriguez, Nam Nguyen, Elizabeth Behrman and James Steck

In previous work, we have shown that our model for a quantum neural network is universal, that is, it can perform any quantum calculation. Bennett showed in the 1970s that any classical calculation can be made reversible (and hence implementable) on a quantum computer, so, it follows that our quantum neural network can also perform any classical calculation. But NISQ devices are severely limited in numbers of qubits. We therefore propose a quantum hybrid neural network, employing a classical layer on top of the quantum processing, both trained with machine learning algorithms. This architecture satisfies the conditions for the universal approximation theorem and therefore can approximate any continuous function on a compact set. We demonstrate its usefulness by showing, in simulation, that such an architecture can calculate the entanglement of formation of an input state of two qubits and can be used to solve classification problems.

#3	**Quantum Multiple Kernel Learning** Seyed Shakib Vedaie, Moslem Noori, Ehsan Zahedinejad and Jaspreet Oberoi

Kernel methods play an important role in machine learning, especially when the aim is to learn from scarce data. The success of kernel methods in machine learning applications relies heavily on the inherent mathematical complexity of a given kernel function. One way to design more-effective and complex kernel functions is to employ a linear or a nonlinear combination of multiple individual kernels to form a combined kernel function. Combining kernels in this way is referred to as multiple kernel learning (MKL). In this work we propose a quantum MKL algorithm for machine learning applications. In particular, we propose a quantum circuit architecture to generate different types of quantum kernel combinations. Our approach has two advantages over the existing classical MKL methods. First, our method uses the power of quantum computing to efficiently estimate the combined kernel for a set of individual classically intractable kernels. Second, our method allows the tuning of each of the individual

kernels in order to achieve a more expressive learning model without having to explicitly compute each of the individual kernels. Our experiments on two binary classification problems—a synthetic dataset and the German credit score dataset—demonstrate the superiority of the proposed method over quantum kernel machines that use a single kernel.

#4	**Quantum State Estimation from Partial Tomography Measurements via Imputation and Ensemble Machine Learning** Onur Danaci, Sanjaya Lohani, Brian T Kirby, Michael Brodsky and Ryan T Glasser

Two-qubit systems usually require 36 coincidence measurements for high-fidelity tomographic reconstruction. We randomly simulated both noiseless and noisy coincidence measurement data for pure and mixed states to deploy a pipeline of stacked generalization of machine learning models for imputation, denoising and state estimation without needing to train a different model for each missing measurement. First, missing measurements are compensated by k-NN imputer. Second, a CNN binary classifier detects whether the model is noisy, if so proceeds to denoising autoencoder. Third, another CNN classifier detects whether the state is pure or mixed. Finally, imputed and denoised partial tomography data proceeds to a stack of 1D & 2D CNN, and XGBoost regression models depending on whether they are pure or mixed. We demonstrated high-fidelity state estimation when multiple measurements are lacking.

#5	**Quantum reservoir computing with a single nonlinear oscillator** Luke Govia, Guilhem Ribeill, William Kalfus, Graham Rowlands, Hari Krovi and Thomas Ohki

Given the omnipresence of noise and error, it remains a daunting task to realize the promise of quantum information processing. Adapting noise-resilient classical computing modalities to quantum mechanics may be a viable path towards near-term applications in the noisy intermediate-scale quantum era. Here, we adapt the neuromorphic computing scheme of reservoir computing to use a quantum system as a reservoir. We propose continuous variable quantum reservoir computing in a single nonlinear oscillator. Through numerical simulation of our model we demonstrate quantum-classical performance improvement, and identify its likely source: the nonlinearity of quantum measurement. Beyond quantum reservoir computing, this result may impact the interpretation of results across quantum machine learning. We study how the performance of our quantum reservoir depends on meta-parameters of the setup, such as Hilbert space dimension, and on realistic experimental considerations, such as noise and finite bandwidth control. We discuss near-term experimental implementations. Our results show that quantum reservoir computing in a single nonlinear oscillator is an attractive modality for quantum computing on near-term hardware.

#6	**Machine learning of noise-resilient quantum circuits** Lukasz Cincio, Kenneth Rudinger, Mohan Sarovar and Patrick Coles

Noise mitigation and reduction will be crucial for obtaining useful answers from near-term quantum computers. In this work, we present a general framework based on machine learning for reducing the impact of quantum hardware noise on quantum circuits. Our method, called noise-aware circuit learning (NACL), applies to circuits designed to compute a unitary transformation, prepare a set of quantum states, or estimate an observable of a many-qubit state. Given a task and a device model that captures information about the noise and connectivity of qubits in a device, NACL outputs an optimized circuit to accomplish this task in the presence of noise. It does so by minimizing a task-specific cost function over circuit depths and circuit structures. To demonstrate NACL, we construct circuits resilient

to a fine-grained noise model derived from gate set tomography on a superconducting-circuit quantum device, for applications including quantum state overlap, quantum Fourier transform, and W-state preparation.

#7	**Quantum Fisher information estimation via hybrid quantum-classical computation** Akira Sone, Jacob Beckey, Marco Cerezo and Patrick Coles

The goal of quantum metrology is to employ quantum coherence or quantum entanglement to better estimate unknown parameters characterizing quantum systems via measurement. The fundamental quantity of interest is quantum Fisher information (QFI), which quantifies the ultimate precision achievable in estimating a parameter a quantum state via the quantum Cramer-Rao bound. Therefore, the QFI can be regarded as a reliability measure of a quantum system as a quantum sensor. Noisy Intermediate-Scale Quantum (NISQ) computers are promising in the near future due to the recent progress in the quantum control and measurement techniques. Variational quantum algorithms are one of the most promising strategies in the NISQ era for a wide of applications. In this presentation, we introduce a variational quantum algorithm for the estimation and the maximization of the QFI of a general quantum state. Our algorithm exploits the relation between the fidelity and QFI in order to estimate the latter, specifically, using bounds on the fidelity based on a truncated fidelity involving the largest eigenvalues and eigenvectors of the relevant quantum states.

#8	**Inverse Design of a Graphene-Based Quantum Transducer via Neuroevolution** Kevin Ryczko, Pierre Darancet and Isaac Tamblyn

We introduce an inverse design framework based on artificial neural networks, genetic algorithms, and tight-binding calculations, capable to optimize the very large configuration space of nano- electronic devices. Our non-linear optimization procedure operates on trial Hamiltonians through superoperators controlling growth policies of regions of distinct doping. We demonstrate that our algorithm optimizes the doping of graphene-based three-terminal devices for valleytronics applica- tions, monotonously converging to synthesizable devices with high merit functions in a few thou- sand evaluations (out of $\simeq$ 23800 possible configurations). The best-performing device allowed for a terminal-specific separation of valley currents with $\simeq$ 93% valley purity. Importantly, the devices found through our non-linear optimization procedure have both higher merit function and higher robustness to defects than the ones obtained through geometry optimization.

#9	**Understanding Boltzmann machines by means of Spin-Glass models** Gorka Muñoz-Gil, Alejandro Pozas-Kerstjens, Miguel Angel García-March, Antonio Acín, Maciej Lewenstein and Przemyslaw R. Grzybowski

We present an efficient method for unsupervised learning using Boltzmann machines (BM).
The method is rooted in the control of the spin-glass properties of the Ising model described by the Boltzmann machine's weights, and allows for very easy access to low-energy configurations. We show how the typical initialisation of BM puts them in such spin-glass and represents an unnecessary bottleneck for their training.
We apply RAPID, the combination of Restricting the Axons (RA) of the model and training via Pattern-InDuced correlations (PID), to learn the Bars and Stripes dataset of various sizes and the MNIST dataset. We show how, in these tasks, RAPID quickly outperforms standard techniques for unsupervised learning in generalization ability. Indeed, both the number of epochs needed for effective learning and the computation time per training step are greatly reduced. In its simplest form, PID allows to

approximate the negative phase of the log-likelihood gradient with no Markov chain Monte Carlo sampling costs at all.

#11	**Variational Quantum State Eigensolver** Marco Cerezo, Kunal Sharma, Andrew Arrasmith and Patrick J. Coles

Extracting eigenvalues and eigenvectors of exponentially large matrices will be an important application of near-term quantum computers. The Variational Quantum Eigensolver (VQE) treats the case when the matrix is a Hamiltonian. Here, we address the case when the matrix is a density matrix ρ. We introduce the Variational Quantum State Eigensolver (VQSE), which is analogous to VQE in that it variationally learns the largest eigenvalues of ρ as well as a gate sequence V that prepares the corresponding eigenvectors. VQSE exploits the connection between diagonalization and majorization to define a cost function $C=\Tr(\tilde{\rho} H)$ where H is a non-degenerate Hamiltonian. Due to Schur-concavity, C is minimized when $\tilde{\rho} = V\rho V^\dagger$ is diagonal in the eigenbasis of H. VQSE only requires a single copy of ρ (only n qubits), making it amenable for near-term implementation. We demonstrate two applications of VQSE: (1) Principal component analysis, and (2) Error mitigation.

#12	**Noise Resilience of Variational Quantum Compiling** Kunal Sharma, Sumeet Khatri, Marco Cerezo and Patrick J. Coles

Variational hybrid quantum-classical algorithms (VHQCAs) are near-term algorithms that leverage classical optimization to minimize a cost function, which is efficiently evaluated on a quantum computer. Recently VHQCAs have been proposed for quantum compiling, where a target unitary U is compiled into a short-depth gate sequence V. In this work, we report on a surprising form of noise resilience for these algorithms. Namely, we find one often learns the correct gate sequence V (i.e., the correct variational parameters) despite various sources of incoherent noise acting during the cost-evaluation circuit. Our main results are rigorous theorems stating that the optimal variational parameters are unaffected by a broad class of noise models, such as measurement noise, gate noise, and Pauli channel noise. Furthermore, our numerical implementations on IBM's noisy simulator demonstrate resilience when compiling the quantum Fourier transform, Toffoli gate, and W-state preparation. Hence, variational quantum compiling, due to its robustness, could be practically useful for noisy intermediate-scale quantum devices. Finally, we speculate that this noise resilience may be a general phenomenon that applies to other VHQCAs such as the variational quantum eigensolver.

#13	**Quantum signal processors for improved imaginary time evolution** Thais Lima Silva, Márcio Taddei and Leandro Aolita

We present two novel efficient quantum algorithms for imaginary-time evolution. Plus, we derive a universal lower bound on the runtime of all such algorithms. One of our algorithms possesses an optimal runtime (i.e. saturates the bound) for large temperatures and a nearly optimal one for small ones, and is well-suited to future quantum computers. The other one features a slightly higher runtime but is ideal for near-term implementations, requiring a single ancillary qubit throughout.

#14	**Phase Diagram Reconstruction of the Bose-Hubbard Model with a Restricted Boltzmann Machine Wavefunction**

Vladimir Vargas-Calderón, Herbert Vinck-Posada and Fabio A. González

Background: Recently, the use of neural quantum states for describing the ground state of many- and few-body problems is increasing because of their high expressivity and ability to handle intractably large Hilbert spaces. Methods based on variational Monte Carlo (VMC) have been proven to be successful in describing the physics of bosonic systems such as the Bose-Hubbard (BH) model. However, this technique has not been systematically tested on the paramter space of the BH model. Moreover, the majority of work has characterised the energy convergence, instead of the more important problem of characterising the state convergence.

Purpose: In our work [1]a, we evaluate the capabilities of VMC with a trial wavefunction given by a Restricted Boltzmann Machine (RBM) to reproduce the quantum ground state of the BH model on several points of its parameter space. The motivation of our work is to test VMC with the RBM ansatz in different Mott lobes and superfluid (SF) regions of the BH phase diagram. We pay attention to the behaviour of the learnt state near the phase transition boundaries, as this region is usually the most challenging for numerical methods. To evaluate the quality of the learnt model, we benchmark our results with ground states found through exact numerical diagonalisation of short 1D chains of sites.

Method: We used the VMC technique introduced by Carleo and Troyer (2017) to learn the ground state of the BH Hamiltonian for several values of hopping and chemical potential parameter, exploring the first two Mott lobes of the BH phase diagram using the NetKet library. We study the energy and state convergence to the exact diagonalised state for 1D systems of 5 and 8 sites. Moreover, we analyse some observables of the system such as the order parameter of the Mott insulator (MI)-SF phase transition, which we choose to be the variance of a local number operator. Also, we examine observables related with the entanglement of the system, such as the linear entropy at the first site of each chain. The study of these properties of the system, as described by the learnt ground state, allows us to assess the accuracy of the VMC method with a RBM wavefunction to represent the ground state of the BH model throughout its parameter space.

Results: Repeatedly, we found that most of the observables measured with the learnt ground state had larger errors at the boundary between the MI and the SF phases. Because of finite-size effects, within the SF regions, plateaus with different excitation manifolds arise. At the boundaries between these plateaus the model also under-performed. Remarkably, the difference between the expected energy of the learnt ground state and the true ground state was minimum at every boundary, even lower than in the regions well within the Mott lobes or well within each plateau in the SF region. Moreover, we found regions in the BH parameter space where the learnt ground state converged to wrong ground states. Nonetheless, we proposed a refining technique that cleaned the learnt ground state, stripping the correct probability distribution of the ground state.

Conclusions: In this work, we systematically tested the capabilities of VMC with a trial ground wavefunction given by a RBM on the one-dimensional BH model. We found that the energy converged very well with low errors at the boundary between the MI and the SF phases. Nonetheless, the learnt ground state overlap with the true ground state was poor at these boundaries. Although we provide a characterisation for this phenomenon, a better understanding is needed of why the method does not perform at these boundaries as well as in other regions of the parameter space.

#15	**Quantum Hamiltonian-Based Models and Variational Quantum Thermalization** Guillaume Verdon, Jacob Marks, Antonio Martinez, Sasha Nanda, Stefan Leichenauer and Jack Hidary

We introduce a new class of generative quantum-neural-network-based models called Quantum Hamiltonian-Based Models (QHBMs). In doing so, we establish a paradigmatic approach for quantum-probabilistic hybrid variational learning, where we efficiently decompose the tasks of learning classical and quantum correlations in a way which maximizes the utility of both classical and quantum processors. In addition, we introduce the Variational Quantum Thermalizer (VQT) for generating the thermal state of a given Hamiltonian and target temperature, a task for which QHBMs are naturally well-suited. The VQT can be seen as a generalization of the Variational Quantum Eigensolver (VQE) to thermal states: we show that the VQT converges to the VQE in the zero-temperature limit. We provide numerical results demonstrating the efficacy of these techniques in illustrative examples. We use QHBMs and the VQT on Heisenberg spin systems, we apply QHBMs to learn entanglement Hamiltonians and compression codes in simulated free Bosonic systems, and finally we use the VQT to prepare thermal Fermionic Gaussian states for quantum simulation.

#16	**Tunable Quantum Neural Networks for Boolean Functions** Viet Pham Ngoc and Herbert Wiklicky

In this paper we propose a new approach to quantum neural networks. Our multi-layer architecture does without the measurements usually emulating the non-linear activation functions that are characteristic of the classical neural networks. Despite this, our proposed architecture is still able to learn any Boolean function. This ability arises from the correspondence that exists between a Boolean function and a particular quantum circuit made out of multi-controlled X gates. This correspondence is built via a polynomial representation of the function called the algebraic normal form. We use this construction to introduce the idea of a generic quantum circuit whose gates can be tuned to learn any Boolean functions. In order to perform the learning task, we have devised an algorithm that leverages the absence of measurements. When presented with a superposition of all the binary inputs of length n, the network can learn the target function in at most n+1 updates.

#17	**Quantum Natural Language Processing on Near-Term Quantum Computers** Konstantinos Meichanetzidis, Stefano Gogioso, Alexis Toumi, Giovanni De Felice, Nicolo Chiappori and Bob Coecke

In this work, we describe a full-stack pipeline for natural language processing on near-term quantum computers, aka QNLP. The language modelling framework we employ is that of compositional distributional semantics (DisCoCat), which extends and complements the compositional structure of pregroup grammars. Within this model, the grammatical reduction of a sentence is interpreted as a diagram, encoding a specific interaction of words according to the grammar. It is this interaction which, together with a specific choice of word embedding, realises the meaning (or ”semantics”) of a sentence. Building on the formal quantum-like nature of such interactions, we present a method for mapping DisCoCat diagrams to quantum circuits. Our methodology is compatible both with NISQ devices and with established Quantum Machine Learning techniques, paving the way to near-term applications of quantum technology to natural language processing.

#18	**Hamiltonian reconstruction as metric for a variational study of the J1J2 model** Kevin Zhang, Samuel Lederer, Kenny Choo, Titus Neupert, Giuseppe Carleo and Eun-Ah Kim

Evaluating the goodness of variational wavefunctions is a hard task due to the large dimensionality of Hilbert space. At the same time, modern methods such as artificial neural networks or variational quantum eigensolvers need accurate evaluation of wavefunctions to facilitate effective development. We propose using a recently developed Hamiltonian reconstruction method for a multi-faceted approach to evaluating wavefunctions. Starting from convolutional neural network (CNN) ansatze trained on a square lattice J1-J2 model, we compare reconstructed Hamiltonians to the original Hamiltonian to evaluate various aspects of the wavefunction. We find that the CNN wavefunctions are systematically better eigenstates of Hamiltonians that 1) are less frustrated, and 2) have easy-axis anisotropy. Also, exclusively in the large J2 regime, the wavefunctions are better eigenstates of Hamiltonians with an antiferromagnetic long-range interaction.

#19	**Online error cancellation using stochastic bandit feedback from spectator qubits** Swarnadeep Majumder, Faris Sbahi, Iman Marvian and Kenneth R. Brown

The biggest challenge in implementing a quantum computer is dealing with noise. Although a series of error mitigation techniques have been proposed in recent years, most do not work well for time-dependent noise processes. In this work, we study the use of spectator qubits to probe the environment and learn about a random noise process affecting our quantum computer. These extra qubits do not take part in the computation and hence can be periodically measured without disturbing the data qubits. In particular, we propose a class of derivative-free optimization methods inspired by the emerging field of online optimization with bandit feedback. Such reinforcement learning methods seek to optimize a structured objective using only random zeroth-order derivative feedback. Specifically, we design a mirror descent based algorithm to maximize average gate fidelity using multi-point feedback and compare to extensions of classic multi-armed bandit algorithms that are agnostic of structure like Thompson sampling. Our noise model is based on a multipartite mixed-unitary channel with an additional source of slow-moving drift. This effectively models both fast varying errors (errors drawn from a distribution between subsequent gates) and slow varying errors (cumulants of the distribution changing in time). We perform numerical simulations demonstrating how our algorithms perform on distinct noise distributions and details of hyperparameter tuning. We also show that our mirror descent algorithm converges to the optimal measurement and correction parameters, in the PAC-learning sense, with asymptotically optimal regret scaling when we make physically motivated assumptions about the error channel.

#20	**Learning to violate Bell inequality with reinforcement learning** Alexey Melnikov

Finding optical setups producing measurement results with a targeted probability distribution is hard as a priori the number of possible experimental implementations grows exponentially with the number of modes and the number of devices. To tackle this complexity, we introduce a method combining reinforcement learning and simulated annealing enabling the automated design of optical experiments producing results with the desired probability distributions. We illustrate the relevance of our method by applying it to a probability distribution favoring high violations of the Bell-CHSH inequality. As a result, we propose new unintuitive experiments leading to higher Bell-CHSH inequality violations than the best

currently known setups. Our method might positively impact the usefulness of photonic experiments for device-independent quantum information processing.

#21	**Certificates of quantum many-body properties assisted by machine learning** Borja Requena, Gorka Muñoz-Gil, Maciej Lewenstein, Vedran Dunjko and Jordi Tura

In physics and optimization, we often encounter computationally intractable tasks. Among the various approaches to tackle such problems, relaxation techniques have been proposed to find lower bounds to the solutions. In this work, we propose a novel approach combining the power of relaxation techniques with deep reinforcement learning to find the best possible bounds given a limited computational budget. We illustrate the viability of the method in the context of finding ground state energy of many-body quantum systems, a paradigmatic problem in quantum physics. We benchmark it against other classical optimization algorithms, such as simulated annealing and breadth first search. Finally, we leverage transfer learning to infer, with a completely unsupervised approach, properties of the physical systems at hand.