Lecture 3: Quantum Machine Learning and Applications of Quantum Computing to HEP

Heather M. Gray UC Berkeley/LBNL Aka: How might this be useful for us?



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CERN Academic Training, March 2021



Outline for the lectures

• Lecture I: Fundamentals

• A brief history, qubits, quantum circuits, qubit technologies

Lecture 2: Quantum computers and quantum algorithms

• Quantum computers today, quantum algorithms, error correction, quantum advantage

Lecture 3: Applications of quantum computing in HEP

• Applications of quantum computing to HEP: simulation, reconstruction and physics analysis; including quantum machine learning



Computing in HEP

- Computing plays a vital role in our successful exploitation of physics results from the LHC
 - Computing is used extensively from detector control, through simulation, to data reconstruction and analysis
- HEP also has a long tradition of being at the forefront of new computing technologies (and even inventing them in certain cases)
 - e.g. the WWW and the grid
- Can quantum computing be useful for HEP?







Outline for Today

- Applications of quantum computing in HEP
 - Simulation
 - Parton shower correlations
 - Lattice QCD
 - Reconstruction
 - Particle tracking
 - Analysis
 - Higgs analyses
 - SUSY search

Progress has been very rapid here... Relying on a mix of published and unpublished results My apologies to anyone who's work I've left out or don't do justice to

Simulation



Reconstruction



Analysis



Simulation



Simulating Parton Shower Correlations

• Idea: exploit entanglement between qubits on a quantum computer to simulate correlations in the parton shower



Bauer et al., arXiv:1904.03196

Toy Model Results



Quantum circuit for the final state radiation algorithm for one of the N steps

Differential cross section as a function of the largest emission angle using IBM Q Compare interference off (blue) to interference on (red)



Lattice QCD Klco et al, arXiv:1803.03326

Quantum-Classical Computation of Schwinger Model Dynamics using Quantum Computers

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We present a quantum-classical algorithm to study the dynamics of the two-spatial-site Schwinger model on IBM's quantum computers. Using rotational symmetries, total charge, and parity, the number of qubits needed to perform computation is reduced by a factor of ~ 5 , removing exponentially-large unphysical sectors from the Hilbert space. Our work opens an avenue for exploration of other lattice quantum field theories, such as quantum chromodynamics, where classical computation is used to find symmetry sectors in which the quantum computer evaluates the dynamics of quantum fluctuations.



Avkhadiev et al, arXiv: 1908.04194

Accelerating lattice quantum field theory calculations via interpolator optimization using NISQ-era quantum computing

A. Avkhadiev,^{1,2} P. E. Shanahan,^{1,2} and R. D. Young³

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The only known way to study quantum field theories in non-perturbative regimes is using numerical calculations regulated on discrete space-time lattices. Such computations, however, are often faced with exponential signal-to-noise challenges that render key physics studies untenable even with next generation classical computing. Here, a method is presented by which the output of smallscale quantum computations on Noisy Intermediate-Scale Quantum era hardware can be used to accelerate larger-scale classical field theory calculations through the construction of *optimized interpolating operators*. The method is implemented and studied in the context of the 1+1-dimensional Schwinger model, a simple field theory which shares key features with the standard model of nuclear and particle physics.

Reconstruction

Track reconstruction studies

- Quantum Annealing x 2
- Quantum Associative Memory
- Quantum Hough Transform
- Quantum Graph Neural Network



Almost all studies here use the <u>trackML</u> dataset Many restrict the multiplicity and/or focus on the central detector region and/or high p_T

Quantum Annealing

- Reformulated track reconstruction as an energy minimisation problem
 - Solve using the D-Wave quantum annealer
 - Solution time doesn't scale with number of tracks
- Implemented QUBO minimisation on D-Wave and study scaling with track multiplicity
 - Inspired from *, but use triplets (3 hits) as the qubits
 - Encode the quality of the triplets based on physics properties. Pair-wise connections b act as constraints (>0) or incentives (<0)
 - Minimizing O means selecting the best triplets to form track candidates



*<u>Stimpfl-Abele & Garrido, Fast track</u> finding with neural networks

Slide credit: L. Linder

Bapst et al, arXiv: 1902.08324

Implementation

- Dataset:
 - trackML dataset
 - barrel, >I GeV, 5+ hits)
- QUBO solvers:
 - qbsolv (D-Wave + simulation)
 - neal (simulation)
- Computers
 - D-Wave 2X (1152 qubits),
 - D-Wave 2000Q (2048 qubits)
 - Fujitsu DA (1025 qubits)





Slide credit: L. Linder

Initial Performance with DWave

Physics performance as a function of occupancy using a D-Wave 2X (qbsolv).









Slide credit: L. Linder

Improved Performance + Digital Annealer

- Further work to improve the purity of the algorithm
 - Extend to expected HL-LHC multiplicities
- Study performance using the Fujitsu Digital Annealer
 - Annealing time is independent of the number of tracks
 - Superior performance to DWave



Density [%]	N _{slice}	DA	neal [sec]	
		CPU time	Anneal time	total time
5	46	0.09	0.29	0.27
10	68	0.15	0.42	0.66
20	71	0.22	0.44	1.29
40	74	0.52	0.45	2.46
60	73	0.94	0.45	4.29
80	74	1.79	0.46	7.49
100	74	3.73	0.45	12.87

<u>Saito et al</u>

Quantum Annealing

- A second implementation of quantum annealing using Hopfield networks for tracking from <u>Zlokapa et al, arXiv</u>: <u>1908.04475</u>
- KDE to estimate connection probability for a pair of hits







<u>Zlokapa et al, arXiv: 1908.04475</u>

Associative Memory



Inspired by ideas for hardware based track triggers

Memory required scales far more slowly with the number of tracks



Slide credit: I. Shapoval

Implementation

- QuAM circuit generators implementing the Trugenberger's initialization and generalized Grover's algorithms.
 - use open-source quantum computing platform, <u>Qiskit</u>
- Supported backends
 - IBM QE cloud-based quantum chips [5Q Yorktown/Tenerife, 14Q Melbourne, 20Q Tokyo]
 - Local/remote noisy simulators



Ex.: complete circuit for retrieving one 2bit pattern

Ex.: complete circuit for retrieving one 2-bit pattern



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Shapoval et al, arXiv:1902.00498

Slide credit: I. Shapoval

Quantum Hough Transform





<u>Chen et al, arXiv:1908.07943</u>

Slide Credit: A. Yadav

Quantum Graph Neural Networks

- <u>GNNs for particle tracking</u> are being developed by the Exa.TrkX collaboration
- Recent <u>studies</u> of the application of QGNNs to particle tracking
 - Hybrid quantum-classical algorithm
 - Encode the hit coordinates as angles
 - Iteratively apply quantum edge and node networks to propagate information to all detector layers
 - Final application of the edge network classifies the segments



arXiv:2003.08126, arXiv:2007.06868.pdf, Talk by Tuysuz at CTD 2020

QGNN Results

- Obtains AUC on 0.8
- Performance decreases as number of iterations increases
 - Attributed to the limited statistics and network simplicity (100 events)

Quantum edge network





Tuysuz et al, arXiv:2007.06868



Analysis



ML on Quantum Computers



Analysis

 $H \rightarrow \gamma \gamma$



Three Higgs analyses One SUSY search



$H \rightarrow \mu \mu$ ATLAS, PLB 812 (2021) 135980



Quantum Machine Learning

- QML lies at the intersection between quantum computing and machine learning
- Usually, we're talking about using quantum computers to analyse classical data
- In many cases, the most promising methods are hybrid classical/quantum approaches
- Both quantum annealers and digital quantum computers have been explored
- Introductory QML <u>textbook</u>
- Recent <u>review article</u> about quantum machine learning in HEP
- Not trying to provide an overview here; rather trying to show examples of studies that have been performed

Don't fall for the hype! - Frank Zickert

Quantum Adiabatic Machine Learning

• CMS $H \rightarrow \gamma \gamma$ search using QAML [arXiv:0104129, arXiv:0001106] using DWave



- <u>Pudenz et al, arXiv:1109.0325</u>
 - Training: identify optimal set of weak classifiers to form strong classifier
 - Testing: evolve strong classifiers to identify anomalous elements

Slide Credit, J.R.Vlimant



$H \rightarrow \gamma \gamma$ Setup

- Dataset: 300k signal; 300k background events
- Training: subsets ranging from 100 to 20k events
- Testing: 100k signal; 100k background
- Key discriminating variables (photon momentum, invariant mass, etc)





- → Evaluate the exact solution of the problem using simulating annealing of the Ising model.
- → Scan for λ, penalty on number of weak classifiers.
- Classification performance depending on the size of the training set.
- Scan on the fraction of exited states included in the classifier.

Slide Credit, J.R.Vlimant

$H \xrightarrow{p_{\tau}^2/(p_{\tau}^1)} \overline{\gamma} \xrightarrow{\gamma} Results$

doi:10.1038/nature24047

$p_T^1 m_{\gamma\gamma}$ Solving a Higgs optimization problem with quantum annealing for machine learning

Alex Mott¹^{†*}, Joshua Job^{2,3*}, Jean-Roch Vlimant¹, Daniel Lidar^{3,4} & Maria Spiropulu¹



QAML with **Zooming**

- Recent extension to these results with the introduction of QAML with zooming
- Idea: Iteratively perform QA to obtain the weights on the weak classifiers continuous
 - Binary search over energy surface using spin up/down outcomes



Results for $H \rightarrow \gamma \gamma$ **on DWave 2X**



Comparison to Simulation

<u>Zlokapa et al, arXiv: 1908.04480</u>



Our program with Quantum Machine Learning

Our Goal:

To perform LHC High Energy Physics analysis with Quantum Machine Learning, to explore and to demonstrate that the potential of quantum computers can be a new computational paradigm for big data analysis in HEP, as a proof of principle

Our present program is to employ the following 3 quantum machine learning methods

- **1. Variational Quantum Classifier Method**
- 2. Quantum Support Vector Machine Kernel Method
- **3. Quantum Neural Network Method**

to LHC High Energy Physics analysis, for example ttH (H $\rightarrow \gamma\gamma$) and H $\rightarrow \mu\mu$ (two LHC flagship analyses).

Sau Lan Wu (U. Wisconsin)

QuantHEP Seminar

November 4 2020

Typically used 100 events and 10 variables

Variational Quantum Classifier

Method 1: Variational Quantum Classifier (VQC)

- 1. Apply feature map circuit $U_{\Phi(\vec{x})}$ to encode input data \vec{x} into quantum state $|\Phi(\vec{x})\rangle$
- 2. Apply short-depth quantum variational circuit W(θ) which is parameterized by gate angles θ
- 3. Measure the qubit state in the standard basis (standard basis: |0>, |1> for 1 qubit; |00>, |01>, |10>, |11> for 2 qubits; ...)
- 4. Assign the label ("signal" or "background") to the event through the action of a diagonal operator f in the standard basis



- During the training phase, a set of events are used to train the circuit W(θ) to reproduce correct classification
- Using the optimized W(θ), an independent set of events are used for evaluation and testing

Sau Lan Wu (U. Wisconsin)

QuantHEP Seminar

November 4, 2020 14

Slide Credit, S.LWu; arXiv:2012.11560.pdf

VQC Results



Similar performance to classical methods



Good agreement between simulation and hardware





arXiv:2012.11560.pdf

Quantum SVM Kernel Method



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QSVM Results

- Improved performance over classical methods
- Good agreement between simulation and hardware
- Impact from noise in the hardware observed



Material courtesy of S.L.Wu, publication coming soon

Hybrid Quantum Neural Network

Method 3: Hybrid Quantum Neural Network (QNN)

We have been developing a hybrid QNN of three layers:



- Classical layer 1: transform input data so that its number of outputs matches number of qubits (PCA is no longer necessary)
- Quantum layer (the core part): encode classical data into a quantum state, apply variational circuit containing trainable parameters, measure the quantum state
- Classical layer 2: convert the measurement of qubits to classification labels

Three layers are trained together to maximize the overall performance

Sau Lan Wu (U. Wisconsin)

QuantHEP Seminar

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QNN Results

IBM hardware



Slightly worse on IBM hardware than in simulation

In simulation, QNN has slightly better performance than DNN



Comparison of different ML methods

ttH (H->γγ)	VQC	QSVM Kernel	QSVM Kernel	QNN	QNN
	IBM	IBM	Amazon	Google	Google
	simulator	simulator	simulator	simulator	simulator
AUC	0.83	0.89	0.89	0.90	0.93
	(100 events	(3200 events	(3200 events	(3200 events	(~0.5 million events
	10 qubits)	10 qubits)	10 qubit)	10 qubits)	13 qubits)

 \sim 9.2 w 20k events, 20 qubits

In most cases, the performance already exceeds the reference classical algorithms

Significant variation between the different ML approaches. Best performance obtained using a QNN on a google simulator with 13 qubits

QML for SUSY Studies



- Input data and iteratively tune the circuit parameters to obtain the desired output
- Output calculation on QC, parameter turning on CC
- Search for chargino pair production via a Higgs boson using SUSY dataset from <u>UCI</u> <u>ML repository</u> (2I + MET)
- I00-I0k events; 3-7 variables

Terashi et al, arXiv:2002.09935.pdf



VQC Circuit



QCL Circuit

QML SUSY Results

 Use two 20 qubit IBM quantum computers and the IBM Qulacs simulator



VQC Results

	Device/Condition	AUC
VQC	Johannesburg Boeblingen QASM simulator	$\begin{array}{c} 0.799 \pm 0.020 \\ 0.807 \pm 0.010 \\ 0.815 \pm 0.015 \end{array}$
QCL	Qulacs simulator $(N_{\text{var}}^{\text{depth}} = 1)$ Qulacs simulator $(N_{\text{var}}^{\text{depth}} = 3)$	0.768 ± 0.082 0.833 ± 0.063

QCL Results



VQC Results



Terashi et al, arXiv:2002.09935.pdf

Incomplete list of other studies for HEP

- Quantum gate optimization for scientific applications: <u>https://arxiv.org/pdf/</u> <u>2102.10008.pdf</u>
- Simulating collider physics on QC: <u>https://arxiv.org/pdf/2102.05044.pdf</u>
- Vertexing with QA: <u>https://arxiv.org/pdf/1903.08879.pdf</u>
- QA for jet clustering: <u>https://journals.aps.org/prd/abstract/10.1103/</u> <u>PhysRevD.101.094015</u>
- Unfolding with QA: <u>https://link.springer.com/article/10.1007/</u> JHEP11(2019)128
- Unfolding to mitigate readout errors: <u>https://www.nature.com/articles/</u> <u>s41534-020-00309-7</u>

Summary

- Quantum computing is an exciting field currently going through a rapid development cycle
 - Major players include a wide range of tech companies and governments around the world
 - A wide range of technologies are being explored including superconducting, trapped ion, photonic, silicon and topological qubits
 - People are particularly excited because
 - Quantum computers may be able to do things that classical computers cannot
 - Quantum computers may be able to solve certain problems far more quickly
 - A recent success was the demonstration of quantum advantage



Conclusion

- Currently available quantum computers have limited numbers of qubits, short coherence times and are very noisy
 - Many problems need to be solved to continue to scale the size and power of quantum computers
- Projections vary wildly about when we might expect (if ever) to have a quantum computer of the size to be more generally useful
- HEP is increasingly becoming constrained by computing resources
 - Increasing dataset sizes, increasing complexity
 - Even more true when planning future colliders
- We also have a long history of being trail blazers in many areas including computing
 - Many interesting studies have been and continue to be performed
 - Will help to determine how quantum computers can be useful for us and also can help to provide difficult problems which can impact design

Thank you!