Abstract of my presentation:
Quantum computing promises an unprecedented ability to solve intractable problems by harnessing quantum mechanical effects such as tunneling, superposition, and entanglement. The Quantum Artificial Intelligence Laboratory (QuAIL) at NASA Ames Research Center is the space agency’s primary facility for conducting research and development in quantum information sciences. QuAIL conducts fundamental research in quantum physics but also explores how best to exploit and apply this disruptive technology to enable NASA missions in aeronautics, Earth and space sciences, and space exploration. At the same time, machine learning has become a major focus in computer science and captured the imagination of the public as a panacea to myriad big data problems. In this talk, we will discuss how classical machine learning can take advantage of quantum computing to significantly improve its effectiveness. Although we illustrate this concept on a quantum annealer, other quantum platforms could be used as well. If explored fully and implemented efficiently, quantum machine learning could greatly accelerate a wide range of tasks leading to new technologies and discoveries that will significantly change the way we solve real-world problems.
Quantum Machine Learning

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Why Quantum Computing at NASA

Data Analysis and Data Fusion

Key: Potential quantum speedup

Anomaly Detection and Decision Making

Air Traffic Management

V&V and optimal sensor placement

Mission Planning and Scheduling, and Coordination

Topologically aware Parallel Computing

Common Feature: Intractable (NP-hard / NP-complete) problems!
QuAIL: Quantum Artificial Intelligence Laboratory

Brief Development Timeline

2000–2011: Occasional NASA research on quantum computing, including seminal papers on adiabatic quantum computing & quantum annealing

Jan 2012: NASA organizes the First Quantum Future Technologies Conference attracting eminent researchers worldwide and participation from companies such as Google and D-Wave Systems

Nov 2012: NASA signs innovative 3-way Non-Reimbursable Space Act Agreement (NRSAA) with Google and USRA

Jan 2013: Site preparations begin at NASA Ames using Center investment funds for installation of D-Wave quantum annealer

Sept 2013: 512-qubit D-Wave 2 system comes on-line at Ames

June 2014: AFRL funding for research in quantum annealing

Aug 2014: IARPA funding for MIT-LL led QEO collaboration among NASA, TAMU, ETH-Z, UC Berkeley, and MIT

July 2015: Upgraded D-Wave 2X quantum annealer comes on-line with over 1000 qubits

Feb 2017: NASA signs NRSAA with Rigetti Computing for collaborative work on their prototype universal quantum processor

April 2017: Latest upgrade underway for D-Wave system with over 2000 qubits

May 2017: NASA to lead T&E effort for IARPA QEO program

QuAIL team has published 40+ papers since 2012
NASA QuAIL Team Focus

**Long Term**
- Determine the breadth and range of quantum computing applications
- Explore potential quantum algorithms and applications of relevance to NASA
- Evaluate, influence, and utilize emerging quantum hardware
  - Develop programming principles, compilation strategies, etc.
  - Characterize the hardware capabilities, noise, etc.
  - Evaluate and implement the most promising NASA applications
- Projections based on fundamental understanding of quantum physics

**Ongoing Efforts**
- Initial target: Quantum Annealing
  - Only significant quantum hardware available are quantum annealers from D-Wave Systems
  - Currently the most prominent quantum heuristic
  - Widely applicable to optimization problems, and sampling for ML
  - Early hardware used to develop intuitions and identify potential
- Near-term target: Emerging quantum computing hardware
  - Small universal quantum systems
  - Advanced quantum annealers
  - Alternative approaches to optimization, sampling for ML, etc.
Foundational Theory of Quantum Annealing

**Simulated Annealing**

(Kirkpatrick et al., 1983)

- **Algorithm:** Start with high temperature; then, gradually reduce intensity of thermal fluctuations to obtain optimal configuration
- Transitions between states via jumping over barriers due to thermal fluctuations

\[ E(\{z\}) \]: Free energy surface (cost function)
\{z\}=configurations in solution space

**Quantum Annealing**

(Finnila et al., 1994, Kadowaki & Nishimori, 1998, Farhi et al., 2001)

- **Algorithm:** Start with large amplitude \( A(\tau) \) responsible for quantum fluctuations; then, gradually turn it off while turning on the cost function of interest \( B(\tau) \)
- Transitions between states via tunneling through barriers due to quantum fluctuations

\[ E(\{z\}, \tau=1) \]
Final state a bit string encoding the solution with probability

\[ E(\{z\}, \tau<1) \]
Quantum states explored by quantum tunneling

\[ E(\{z\}, \tau=0) \]
Initialize in an easy to prepare full quantum superposition
NASA Quantum Research Approach

**ROBUST QUANTUM ANNEALING**
- Tailored problems to show quantum enhancement
- Hidden bottlenecks of large-scale problems
- Error suppression techniques
- Optimal parameter setting
- Annealing theory of embedded problems
- Phase transitions in application problems
- Design of new application-focused QA architectures

**APPLICATION PROBLEMS**

**ADVANCED PROGRAMMING**
- Device calibration techniques
- Study of annealing in 1D chains
- New embedding techniques
- Insights into and intuitions for quantum heuristics
- Future architectural design elements
- Performance estimators
- QA solvers for complex planning and scheduling problems
- Graph-based fault-detection problems
- Machine Learning and Artificial Intelligence

**NASA**
D-Wave System Hardware

- Collaboration with Google and USRA led to installation of system at NASA Ames in 2013
- Started with 512-qubit Vesuvius processor (currently upgrading to 2000-qubit Whistler)
- 10 kg metal in vacuum at ~15 mK
- Magnetic shielding to 1 nanoTesla
- Protected from transient vibrations
- Single annealing takes 20 μs
- Typical run of 10,000 anneals (incl. reset & readout takes ~4 sec)
- Uses 12 kW of electrical power

Focused on solving discrete optimization problems using quantum annealing
D-Wave System Capability

The system solves only one binary optimization problem:

Given \( \{ h_j, J_{ij} \} \), find \( \{ s_k = \pm 1 \} \) that minimizes

\[
\xi(s_1, \ldots, s_N) = \sum_{j=1}^{N} h_j s_j + \sum_{i,j \in E} J_{ij} s_i s_j
\]
### Vesuvius to Washington to Whistler

<table>
<thead>
<tr>
<th>D-Wave Two</th>
<th>D-Wave 2X</th>
<th>D-Wave 2000Q</th>
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<tbody>
<tr>
<td><strong>512</strong> (8x8x8) qubit “Vesuvius” processor</td>
<td><strong>1152</strong> (8x12x12) qubit “Washington” processor</td>
<td><strong>2048</strong> (8x16x16) qubit “Whistler” processor</td>
</tr>
<tr>
<td><strong>509</strong> qubits working – 95% yield</td>
<td><strong>1097</strong> qubits working – 95% yield</td>
<td><strong>2038</strong> qubits working – 97% yield</td>
</tr>
<tr>
<td><strong>1472 J</strong> programmable couplers</td>
<td><strong>3360 J</strong> programmable couplers</td>
<td><strong>6016 J</strong> programmable couplers</td>
</tr>
<tr>
<td><strong>20 mK</strong> max operating temperature (<strong>18 mK</strong> nominal)</td>
<td><strong>15 mK</strong> max operating temperature (<strong>13 mK</strong> nominal)</td>
<td><strong>15 mK</strong> max operating temperature (<strong>nominal to be measured</strong>)</td>
</tr>
<tr>
<td><strong>5% and 3.5%</strong> precision level for ( h ) and ( J )</td>
<td><strong>3.5% and 2%</strong> precision level for ( h ) and ( J )</td>
<td><strong>To be measured</strong></td>
</tr>
<tr>
<td><strong>20 us</strong> annealing time</td>
<td><strong>5 us</strong> annealing time (4X better)</td>
<td><strong>5 us</strong> annealing time</td>
</tr>
<tr>
<td><strong>12 ms</strong> programming time</td>
<td><strong>12 ms</strong> programming time</td>
<td><strong>9 ms</strong> programming time (25% better)</td>
</tr>
<tr>
<td><strong>New:</strong> anneal offset, pause, quench</td>
<td></td>
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</tr>
<tr>
<td><strong>6 graph connectivity per qubit</strong></td>
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</table>
Programming the D-Wave System

1. **Map the target combinatorial optimization problem into QUBO**
   No general algorithms but smart mathematical tricks (penalty functions, locality reduction, etc.)

   \[
   \alpha_{ijk} z_i z_j z_k
   \]

   \[
   \alpha_{ij} y_i z_k + \beta_{ijk} (3y_j - 2z_i y_j - 2z_j y_i + z_i z_j)
   \]

   \[
   \sum_{ij} Q_{ij} z_i z_j \rightarrow \\
   \sum_i h_i s_i + \sum_{i,j} J_{ij} s_i s_j
   \]

   **Mapping not needed for random spin-glass models**

2. **Embed the QUBO coupling matrix in the hardware graph of interacting qubits**
   D-Wave qubit hardware connectivity is a Chimera graph, so embedding methods mostly based on heuristics

   \[
   Q_{ij} =
   \]

   **Embedding not needed for native Chimera problems**

3. **Run the problem several times and collect statistics**
   Use symmetries, permutations, and error correction to eliminate the systemic hardware errors and check the solutions

   **Performance can be improved dramatically with smart pre-/post-processing**

   **Probability**

   **Solution’s energy/cost**
Mapping to QUBO: Graph Coloring Example

Graph Coloring Problem:
Assign one of $k$ colors to each vertex so that no two vertices sharing an edge have the same color.

Binary variable:

$$x_{v,c} = \begin{cases} 1 & \text{vertex } v \text{ with color } c \\ 0 & \text{vertex } v \text{ not with color } c \end{cases}$$

Violation of requirements encoded as cost:

- (1) unique assignment: Each vertex $v$ must be assigned exactly one color:

$$H^{(unique)}_v = (\sum_{c \in C} x_{v,c} - 1)^2 \iff \sum_{c \in C} x_{v,c} = 1$$

- (2) Connected vertices cannot use the same color:

$$H^{(exclude)}_{v,v',c} = x_{v,c}x_{v',c} \quad \text{if} \quad vv' \in E$$

Final QUBO form:

$$H = \sum_v H^{(unique)}_v + \sum_{v,v' \in E} \sum_c H^{(exclude)}_{v,v',c}$$

$H = 0$ corresponds to a valid coloring.
Embedding the QUBO

Embed a triangle onto a bipartite graph

original QUBO hardware connectivity QUBO embedded

\[
H_0 = J_{12}x_1x_2 + J_{23}x_2x_3 + J_{13}x_1x_3 \\
H_1 = J_{12}x_{1a}x_2 + J_{23}x_2x_3 + J_{13}x_{1b}x_3 + J_{\text{Ferro}}x_{1a}x_{1b}
\]

Strong, but not too strong, ferromagnetic coupling between physical qubits \(x_{1a}\) and \(x_{1b}\) encourages them to take the same value, thus acting as a single logical qubit \(x_1\)

Embedding a realistic problem instance:
Physical qubits on each colored path represent one logical qubit

\(H_0\) and \(H_1\) have the same ground state but the energy landscape of the search space differs

Current research investigation: How best to set the magnitude of these “strong” couplings to maximize probability of success
Current NASA Research in Applications

**Complex Planning and Scheduling**

- General **Planning Problems** (e.g., navigation, scheduling, asset allocation) can be solved on a quantum annealer.
- Developed a quantum solver for **Job Shop Scheduling** that pre-characterizes instance ensembles to design optimal embedding and run strategy – tested at small scale (6x6) but potentially could solve intractable problems (15x15) with 10x more qubits.

**Graph-based Fault Detection**

- Analyzed simple graphs of **Electrical Power Networks** to find the most probable cause of multiple faults – easy and scalable QUBO mapping, but good parameter setting (e.g., gauge selection) key to finding optimal solution – now exploring digital circuit **Fault Diagnostics and V&V**.

**Graph Isomorphism**

- **Subgraph Matching Problems** are common in applications of interest to the intelligence community – similarly, finding **Longest Matching Sequences** important in genomics and bioinformatics.
Current NASA Research in Quantum Physics

Calibration of Quantum Annealers

- Developed technique to determine and correct residual persistent biases in the programmable parameters of quantum annealers (h and J) – correction significantly improves performance and reliability (reduction in variability)

- First realistic noise analyses show how low-frequency noise dramatically affects the performance of quantum annealers – results being used to design hardware improvements

- Limited hardware connectivity makes embedding challenging – good runtime parameters determined by considering the nature and dynamics of chains – quick scans can be used to predict performance of extensive scans

- Small instances of hard problems at phase transitions in combinatorial optimization are intractable – they can be designed by looking at solvability phase transitions

- Predict tractability of application problems by studying the scaling of energy gaps and density of bottlenecks in spin glass phase
Quantum annealing capabilities

1) As a discrete optimization solver:

Given \( \{h_j, J_{ij}\} \), find \( \{s_k = \pm 1\} \) that minimizes

\[
\xi(s_1, \ldots, s_N) = \sum_{j=1}^{N} h_j s_j + \sum_{i,j \in E} J_{ij} s_i s_j
\]

NP-hard problem

Potential NASA applications:
- planning
- scheduling
- fault diagnosis
- graph analysis
- communication networks, etc.

QUBO: Quadratic Unconstrained Binary Optimization (Ising model in physics jargon).

2) As a physical device to sample from Boltzmann-like distributions:

\[
P_{Boltzmann} \propto \exp\left[ -\xi(s_1, \ldots, s_N)/T_{eff} \right]
\]

\[\langle v_i h_j \rangle_{p(h,v)}\]

Computationally bottleneck

Early work:

Follow-up work:

Our work: Benedetti et al. PRA 94, 022308 (2016)
- We provide a robust algorithm to estimate the effective temperature of problem instances in quantum annealers.
- Algorithm uses the same samples that will be used for the estimation of the gradient

Potential NASA applications:
- machine learning (e.g., training of deep-learning networks)

RBM

Widely used in
generative unsupervised learning

Visible units

Hidden units
Unsupervised learning relies on sampling

**Lesson 1:** Move to intractable problems of interest to ML experts (e.g., generative models in unsupervised learning). Quantum advantage in near term.

“Unsupervised learning [... has] been overshadowed by the successes of purely supervised learning. [... We] expect unsupervised learning to become far more important in the longer term. Human and animal learning is largely unsupervised: we discover the structure of the world by observing it, not by being told the name of every object.”


“In the context of the deep learning approach to undirected modeling, it is rare to use any approach other than Gibbs sampling. Improved sampling techniques are one possible research frontier.”


“Most of the previous work in generative models has focused on variants of Boltzmann Machines [...] While these models are very powerful, each iteration of training requires a computationally costly step of MCMC to approximate derivatives of an intractable partition function (normalization constant), making it difficult to scale them to large datasets.”

Mansimov, Parisotto, Ba, Salakhutdinov, ICLR 2016
Unsupervised learning (generative models)

Learn the “best” model distribution that can generate the same kind of data

Example application: Image reconstruction

Learning algorithm

MODEL

\( P(\text{Image}) \)

NO LABELS

DATASET

Reconstructed image

LEARNED MODEL

\( P(\text{Image}) \)

Damaged image
**Supervised learning** (discriminative models)

Learn the “best” model that can perform a specific task

**MODEL**

\[ P(\text{Label} \mid \text{Image}) \]

Learning algorithm

**DATASET**

| 26624 | 98 | 66 | 175 |

Example application:

*Image recognition*

Predicted label

**LEARNED MODEL**

\[ P(\text{Label} \mid \text{Image}) \]

Image to be recognized
A near-term approach for quantum-enhanced machine learning

Lesson 2: Hybrid approaches for generative modeling in unsupervised machine learning.

LEARNING
Stochastic gradient descent

\[ \Theta^{t+1} = \Theta^t + \nabla \left[ \mathcal{L}(\Theta) \right] \]

PREDICTIONS

\[ \mathcal{F}[P(s|\Theta)] \]

Hard to compute
Estimation assisted by sampling from quantum computer

Data
\[ s = \{s_1, \ldots, s^D\} \]

Computationally bottleneck

\[ \langle v_i u_j \rangle_{p(v,u)} \]

Where,

\[ p(v,u) = \frac{e^{-E(v,u|\theta)/T_{eff}}}{Z(\theta)} \]

Ex.: Restricted Boltzmann Machines (RBM)

Visible units, \( v \)

Hidden units, \( u \)

Widely used in unsupervised learning

Challenges solved:


Quantum-assisted unsupervised learning on digits

OptDigits Datasets

Dataset: Optical Recognition of Handwritten Digits (OptDigits)
Quantum-assisted unsupervised learning on digits

OptDigits Datasets

Dataset: Optical Recognition of Handwritten Digits (OptDigits)
Quantum-assisted unsupervised learning on digits

Overcoming the curse of limited connectivity in hardware.

46 fully-connected logical (visible) variables

42 for pixels + 4 to one-hot encode the class (only digits 1-4)

- Are the results from this training on 940 qubit experiment meaningful?
- Is the model capable of generating digits?

Quantum-assisted unsupervised learning on digits

Human or (quantum) machine? (Turing test)

Dataset: Optical Recognition of Handwritten Digits (OptDigits)

Results from experiments using 940 qubits, without post-processing. The hardware-embedded model represents a 46 node fully connected graph.

A near-term approach for quantum-enhanced machine learning

Challenges of the hybrid approach:

- Need to solve classical-quantum model mismatch

Training Method: Stochastic gradient ascent

\[ \sum_{v \in S} \frac{\partial \ln L(\theta|v)}{\partial w_{ij}} \propto \langle v_i h_j \rangle_{\text{data}} - \langle v_i h_j \rangle_{\text{model}} \]

Fully visible models

- Robustness to noise, intrinsic control errors, and to deviations from sampling model (e.g., Boltzmann)

- Curse of limited connectivity – parameter setting

How about large complex datasets with continuous variables? All previous fail to do that (fully quantum and hybrid here)

No progress in five years since QA sampling was proposed as a promising application.

Perspective on quantum-enhanced machine learning

- New hybrid proposal that works directly on a low-dimensional representation of the data.

\[
i\hbar \frac{d\hat{\rho}_\theta(t)}{dt} = [\hat{H}_\theta, \hat{\rho}_\theta]
\]

Perspective on quantum-enhanced machine learning

- New hybrid proposal that works directly on a low-dimensional representation of the data.

Experimental implementation of the QAHM

Experiments using 1644 qubits (no further postprocessing!)

Max. CL = 43

Lesson 1: Focus on the hardest problems of interest to ML experts (e.g., generative models in unsupervised learning).
Quickest path to demonstrating quantum advantage in the near-term

Lesson 2: Focus on novel hybrid quantum-classical approaches.
Cope with hardware constrains. Exploitation of available quantum resources

Conclusions

• Understanding and harnessing the fundamental power of quantum computing is a formidable challenge that requires:
  – New insights in physics and mathematics
  – Innovations in computer and computational science
  – Breakthroughs in engineering design to produce robust, reliable, scalable technologies

• NASA QuAIL team has successfully demonstrated that discrete optimization problems can be run on quantum annealers
  – Effectively using such systems needs judicious mapping, embedding, execution strategies

• Exciting decade in quantum computing ahead of us
  – Compilation and performance capabilities of today’s annealers are improving rapidly
  – New and better quantum algorithms, particularly quantum heuristics, are emerging
  – Small-scale universal quantum computers are becoming available

ENIAC (1946), the first “general-purpose” computer

The task of taking a problem and mapping it onto the machine was complex, and usually took weeks. After the program was figured out on paper, the process of getting the program "into" ENIAC by manipulating its switches and cables took additional days. This was followed by a period of verification and debugging […] (source: http://en.wikipedia.org/wiki/ENIAC)