**What are the major goals of the project?**

Two overarching goals were listed in the proposal: (1) explore the fundamental nature of the claimed quantum annealing behavior and confirm that a wide range of configuration spaces (Markov Random Fields) trained with a variety of application-relevant data) have this property of finding the so-called ‘difficult to find’ local valleys (LVs); (2) apply this behavior to Deep Graphical Models to achieve superior classification and pattern reconstruction accuracy.

**\* What was accomplished under these goals and objectives (you must provide information for at least one of the 4 categories below)?**

Major Activities:

Classical training of RBMs.

Classical search for Local Minima in the RBM Energy Function.

Optimization of RBM embedding into the D-Wave hardware.

RBM-based search for the Ground State and the Local Minima.

MSU and Temple worked on preparing contemporary ML datasets and using RBM for contemporary ML datasets.

Specific Objectives:

Objective 1: confirm the behavior of the D-Wave for graphs and datasets that are more complex than those explored in the pre-proposal work.

Task 1 (nearly completed) – use the D-Wave to find unfamiliar local valleys missed by even a prohibitively long classical search.

Task 2 (nearly completed) – separate the most promising of those local valleys by statistical analysis using a set of criteria.

Task 3 (initiated) – statistically compare basins of attraction for otherwise similar local valleys concerning the size of their basins of attraction.

Objective 2: Develop a hybrid classical-quantum (HCQ) sampling algorithm for RBM training

Task 1 (nearly completed) – develop an approach for embedding large-size graphs in the QAC hardware.

Objective 3: Apply quantum annealing computer to contemporary machine learning problems.

Significant Results:

Objective 1:

Our investigation confirmed observations from the latest publications in the field – the D-Wave quantum annealer improves concerning the time-to-solution when doing its primary job – searching for the ground state. However, we are confirming our preliminary observation that this also means a deteriorated potential for using the D-Wave to obtain a representative, diverse sample from probability distributions. The preliminary used by us criterion of the sample quality was the number of different local valleys found by the D-Wave compared to the classical MCMC. Compared to our pre-proposal experiments on the Chimera D-Wave hardware, the Pegasus hardware consistently provides fewer local valleys compared to the classical search.

We considered a new hypothesis that a reduced annealing time while complicating the discovery of the ground state, should produce a more diverse sample. Experiments with the annealing time remain inconclusive; however, no apparent benefits have been observed. A more statistically-reliable investigation will be required.

Concerning the statistical analysis of the relative “importance” of the local valleys found by the classical vs. the D-Wave search, the results were qualitatively similar to what had been observed in the pre-proposal work on much smaller graphs. The good news was that most of those higher numbers of the local valleys found by the classical search but missed by the D-Wave are higher-energy, lower-probability (i.e., not representative) states. Concerning the states more critical for a high-quality sample, the D-Wave and the classical search miss many local valleys found by the other. This observation preliminary confirmed our central hypothesis explaining that the lack of significant improvements in the D-Wave-based training compared to the classical training, as reported by many research groups, preliminary supported the merits of our main focus on the hybrid classical-quantum training.

Objective 2:

We developed procedures to use graph sizes of significantly higher dimensionality than in the pre-proposal work. The Pegasus architecture of the D-Wave allowed us to move from 64 RBM visible units and incomplete RBM connectivity to (currently) 144 visible units (pixels of the image) and complete RBM connectivity.

Our approach to testing the adequacy of embedding was based on using classically trained (no use of QC) RBMs and applying the D-Wave to reconstruct the classification label by finding the ground state of a model with qubits corresponding to visible RBM units clamped to each of the training patterns. With proper optimization, we observed that the classification error was similar to that from the classical testing (without the D-Wave), which indicated sufficiently precise embedding. This embedding is ready for future experiments with hybrid classical-quantum RBM training algorithms.

Objective 3:

Picone to add … .

Key outcomes or Other achievements:

N/A

**\* What opportunities for training and professional development has the project provided?**

Training for graduate students (as listed in the personnel section).

**\* Have the results been disseminated to communities of interest? If so, please provide details.**

Dissemination products are in the process of preparation and submission.

**\* What do you plan to do during the next reporting period to accomplish the goals?**

Finish Objective 1 – Confirm that the previously observed behavior of the D-Wave for graphs and datasets that are more complex than those explored in the pre-proposal work. Specifically, concerning finishing Task 1 - conduct a more statistically reliable investigation of a possible benefit of a shorter annealing time on the D-Wave’s ability to find a larger than otherwise number of distinct high probability local valleys.

Finish Task 3 – statistically compare basins of attraction for otherwise similar local valleys concerning the size of their basins of attraction. Submit a journal manuscript to Quantum Information Processing.

Continue working on Objective 2 - develop a hybrid classical-quantum (HCQ) sampling algorithm for RBM training. Specifically, finish Task 1 – develop an approach for embedding larger-size graphs in the QAC hardware. We have reasons to deprioritize Task 2 until the third year. Instead, we will prioritize work on Task 3 – develop training algorithms for RBM, based on a hybrid classical-quantum sampling algorithm to achieve improvements beyond the mere speed up of nondirected generative model training.

Objective 3 – Picone to provide input……

**Products**

**Books**

None

**Book Chapters**

None

**Inventions**

None

**Journals or Juried Conference Papers**

None.

**View all journal publications currently available in the NSF Public Access Repository for this award.**

The results in the NSF Public Access Repository will include a comprehensive listing of all journal publications recorded todate that are associated with this award.

**Licenses**

None

**Other Conference Presentations / Papers**

None

**Other Products**

None

**Other Publications**

None

**Patent Applications**

None

**Technologies or Techniques**

None

**Thesis/Dissertations**

None

**Websites or Other Internet Sites**

None

**Participants/Organizations**

|  |  |  |  |
| --- | --- | --- | --- |
| **What individuals have worked on the project?Name** | **Most Senior Project Role** |  | **Nearest Person Month Worked** |
|  |  |  |  |
| Khan, Samee | PD/PI | 2 |
| Picone, Joseph | Co PD/PI |  |
| El Yazizi, Abdelmoula  | Student | 12 |
| Ellenberger, Kenzie | Student | 12 |
|  |  |  |
|  |  |  |
|  |  |  |

**What other organizations have been involved as partners?**

None

**Full details of organizations that have been involved as partners:**

Mississippi State University

Temple University

**Were other collaborators or contacts involved? If so, please provide details.**

N/A

**Impacts**

**What is the impact on the development of the principal discipline(s) of the project?**

New understanding of the limitations of quantum annealers (or at least the D-Wave in particular) for sampling from complex probability distributions. The main new observation concerning that is that new generations of quantum annealing hardware, while showing well-documented in the literature improvements in the main task – finding the ground state – are likely to not improve concerning the sampling applications. This may justify hybrid approaches to sampling.

**What is the impact on other disciplines?**

None

**What is the impact on the development of human resources?**

Graduate students have received valuable guidance on the state of the art QC topics.

**What was the impact on teaching and educational experiences?**

Graduate students received individual educational experiences.

**What is the impact on physical resources that form infrastructure?**

N/A

**What is the impact on institutional resources that form infrastructure?**

N/A

**What is the impact on information resources that form infrastructure?**

N/A

**What is the impact on technology transfer?**

N/A

**What is the impact on society beyond science and technology?**

N/A

**What percentage of the award's budget was spent in a foreign country?**

N/A

**Changes/Problems**

**Changes in approach and reason for change**

So far, the main hypotheses of the proposal about the behavior of the newer-generation quantum hardware (the Pegasus D-Wave quantum annealer) are being confirmed. There have been no reasons for change.

**Actual or Anticipated problems or delays and actions or plans to resolve them**

None.

**Changes that have a significant impact on expenditures**

The vendor’s requirement of a minimum commitment to purchasing the D-Wave time justified our enhanced due diligence and care in the preparational steps, which was done using the free monthly time offered by the D-Wave (1 min per user). A spike in the expenditures for the D-Wave time is planned to start in August.

**Significant changes in use or care of human subjects**

None.

**Significant changes in use or care of vertebrate animals**

None.

**Significant changes in use or care of biohazards**

None.

**Change in primary performance site location**

None.

**Special Requirements**

**Responses to any special reporting requirements specified in the award terms and conditions, as well as anyaward specific reporting requirements.**

N/A