Anomaly Detection in Gamma Spectra Using Hopfield Neural Network with B-SAT and Grover’s Algorithm on a Quantum Computing Simulator

Consortium on Nuclear Security Technologies (CONNECT)

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Abstract

Environmental screening of gamma radiation consists of detecting weak nuisance and anomaly signal in the presence of strong and highly varying background. In a typical scenario, a mobile detector-spectrometer continuously measures gamma radiation spectra in short, e.g., one-second, signal acquisition intervals. In principle, gamma radiation sources can be detected and identified by their unique spectral lines. However, detecting sources from data measured in a search scenario is difficult due to the highly varying background because of naturally occurring radioactive material (NORM), and low signal-to-noise ratio (S/N) of spectral signal measured during one-second acquisition intervals. In recent prior work, we have developed a Hopfield Neural Network (HNN) in conjunction with an image processing algorithm to detect a weak signal anomaly hidden among the highly fluctuating background spectra. The objective of this work is to explore quantum computing methods to increase the speed of HNN. The approach is based on the Grover’s search algorithm in conjunction with a 3-SAT problem formalism. The Grover’s algorithm is implemented on a quantum computing simulator using Qiskit software. Performance of HNN algorithm is benchmarked using search data from an environmental screening campaign, where the anomaly is a subset of measurements containing a $^{137}$Cs source. Results indicate that using Grover’s algorithm on a quantum simulator reduces runtime of HNN by two orders of magnitude.
1. Introduction

Environmental screening of gamma radiation consists of detecting weak nuisance and anomaly signal in the presence of strong and highly varying background. In a typical scenario, a mobile detector-spectrometer continuously measures gamma radiation spectra in short, e.g., one-second, signal acquisition intervals. In principle, gamma radiation sources can be detected and identified from the measured data by their unique spectral lines. However, detecting sources from data measured in a search scenario is difficult due to the highly varying background because of naturally occurring radioactive material (NORM), and low signal-to-noise ratio (S/N) of spectral signal measured during one-second acquisition intervals [1-3].

In recent prior work, we have developed a Hopfield Neural Network (HNN) in conjunction with an image processing algorithm to detect a weak signal anomaly hidden among the highly fluctuating background spectra [4]. Performance of HANN algorithm was benchmarked in detection of orphan sources in data sets containing measurements of $^{137}$Cs and $^{131}$I isotopes, respectively. The first dataset contained 4265 one-second spectra from a NaI scintillation detector, including 95 one-second spectra of $^{137}$Cs source. The second dataset contained 5827 one-second spectra from a NaI scintillation detector, including 88 one-second spectra of $^{131}$I source. Both datasets contained 1024 channels ranging from 0 to 3000keV. Performance accuracy of HNN was ranked with $F_1$ score, which yielded 89% and 95.5% for the two databases, respectively. Runtime of HNN was 5.1s and 7.5s for the two databases, respectively.

In this report, we investigate the use of quantum computing methods to increase the runtime of HNN [5]. The approach to HNN solution consists using a 3-SAT problem formalism with Grover’s search algorithm. The 3-SAT problem is a special case of a Boolean satisfiability (B-SAT) problem, which determines if there exists an interpretation that satisfies a given Boolean formula [6]. Grover’s search algorithm allows to search for a particular pattern in an unsorted list [7]. In a classical scenario with $N$ items in a dataset, it would take on average of $O(N)$ queries to sort the database. However, utilizing Grover’s search algorithm only takes $O(\sqrt{N})$ queries. Grover’s algorithm finds possible combinations, and the ones that satisfy the 3-SAT equation are solutions of HNN. In this work, Grover’s algorithm is implemented with Qiskit quantum computing simulator [8]. Figure 1 shows the flow chart for 3-SAT and Grover’s algorithm solution of HNN.

![Figure 1 – Flow chart of HNN solution with B-SAT formalism and Grover’s search algorithm](image)

Create 3SAT problem

Search for solutions with Grover's Algorithm

Solution vectors are reflected

Amplitude Amplification

Input Solutions into Hopfield Network

Grover's searches for solutions

Solution vectors are reflected again
2. Boolean Satisfiability (B-SAT) Formalism

A 3-SAT is a special case of the Boolean satisfiability (B-SAT) problems. For a given Boolean expression, B-SAT determines if there exists an interpretation that satisfies this equation. Boolean expression consists of variables, operators AND (conjunction ∧), OR (disjunction ∨), NOT (negation¬), and parentheses. A formula is said to be satisfiable if it can be made TRUE by assigning appropriate logical values (TRUE or FALSE) to its variables. The Boolean expression for the 3-SAT problem consists of three variables:

\[ f(v_1v_2v_3) = (\neg v_1 \lor \neg v_2 \lor \neg v_3) \land (\neg v_1 \lor v_2 \lor \neg v_3) \land (v_1 \lor \neg v_2 \lor \neg v_3) \land (\neg v_1 \lor v_2 \lor v_3) \]

(1)

The solution for 3SAT problem is represent in Table 1. Each pattern of solution corresponds to an anomaly solution in HANN.

<table>
<thead>
<tr>
<th>(v_1)</th>
<th>(v_2)</th>
<th>(v_3)</th>
<th>(f)</th>
<th>Comment</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
<td>Solution</td>
</tr>
<tr>
<td>0</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>Not a solution (f) is false</td>
</tr>
<tr>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>Not a solution (f) is false</td>
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<td>0</td>
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<td>Solution</td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>Not a solution (f) is false</td>
</tr>
</tbody>
</table>

The 3-SAT Boolean expression can be coded in a DIMACS CNF file format [9]. Figure 2 shows the text of the of DIMACS CNF file. The first line is a comment that describes the type of file and the type of B-SAT problem. The second line indicates that the input is of CNF format. The numbers 3 and 5 indicate the exact number of variables and clause that appear in the Boolean expression. Each line containing numeric values corresponds to a clause. The numbers within each clause line represent the variables in the Boolean expression equations. Negative numbers are indicated with a “minus sign” in front of the corresponding variables.
Figure 2 – Example of DIMACS file format

c example DIMACS CNF 3-SAT
p cnf 3 5
-1 -2 -3 0
1 -2 3 0
1 2 -3 0
1 -2 -3 0
-1 2 3 0
3. Grover’s Search Algorithm

A search algorithm for an unsorted database of size $N$, on a conventional classical computer scales as $O(N)$. Grover’s search algorithm on a quantum computer scales as $O(\sqrt{N})$. In this work, we implement the Grover’s algorithm on Qiskit quantum computing simulator [7]. The data on the quantum computer has to be structured in a quantum oracle, which converts classical data to quantum qubits (qubits) representation of the data, and performs superposition by using a set of Hadamard gates. Figure 3 shows the quantum circuit oracle with 2 qubits created with Qiskit software.

![Quantum Circuit Oracle](image)

**Figure 3** – Amplification quantum oracle circuit in Qiskit

The structure of the Grover’s algorithm consists of three steps. The first step involves uniform superposition to amplify an item in the database. Amplitude amplification is shown in Figure 3. In the two dimensional plane in the left panel of Figure 3, $|w>$ represents the winner item or solution of the search problem, and $|s'>$ that corresponds to the initial state. The vector $|s>$ is given as

$$|s> = \sin \theta |w> + \cos \theta |s'>$$

(2)

The right panel of Figure 3 shows the database of N elements, where the winner item $|w>$ is colored on purple.

![Amplitude Amplification](image)

**Figure 4** – Amplitude amplification of the vector $|s>$. 

8
The second step involves oracle reflection $U_f$ of the state $|s\rangle$. This is depicted in Figure 4. Reflection of the state $|s\rangle$ in the 2D plane is shown in the left panel of Figure 4, where the reflected state in the quadrant IV of the plane. The right panel of Figure 4 shows amplitude reflection of the item in the database. The quantum circuit created with Qiskit software to perform the reflection operation is shown in the bottom panel.

![Reflection U](image)

**Figure 5** – State reflection and oracle reflection circuit in Qiskit

The third step is an additional reflection $U_s$ of the state $|s\rangle$. This transformation reflects the state back to quadrant I of the plane, and moves the vector closer to the winner item $|w\rangle$. Figure 5 displays the second reflection in the 2D plane (left panel), and as the feature of the item in the database (right panel). The quantum circuit for the second reflection, shown in the bottom panel of Figure 6, is implemented with a set of Hadamard gates.
Steps 2 and 3 are repeated several times until state $|s\rangle$ approximates $|w\rangle$ sufficiently close. The complete circuit performing all steps of the Grover’s algorithm is shown in Figure 6.

**Figure 6** – State second reflection and diffuser circuit representation in Qiskit

**Figure 7** – Complete circuit depiction of Grover’s search algorithm in Qiskit
4. HANN Solution with B-SAT and Grover’s Algorithm in Qiskit

The approach to find HNN solution consists using a 3-SAT problem formalism with Grover’s search algorithm. The measurement data is a 2D matrix, where one dimension is gamma ray energy (0 to 3000keV binned into 1024 channels), and the other dimension is the number of measurements or total time (measurements taken every second). The 2D matrix values are counts per second per spectral channel. Interactions between HNN neurons have units that take on values [1,-1]. To use HNN on a data set requires conversion of data to binary threshold HNN units. This is accomplished by converting the measurement data into a grayscale intensity image, thresholding and normalizing the data to the set of binary values [1,0], and then converting the zero values to -1’s. Samples from each spectrum of data matrix are taken as patterns for the 3-SAT problem. Satisfiability of the Boolean expression corresponds to anomaly detection with HNN. To represent Hopfield data patterns for the 3-SAT formalism, we create a DIMACS CNF file to interface with the Grover’s algorithm implemented with Qiskit Aqua library tools.

The following steps describe the process utilized to apply Groover’s algorithm. A phase Oracle is created that reads the Boolean expression from the DIMACS CNF file. The command lines and the phase oracle circuit created with Qiskit are shown in Figure 8.

```python
oracle = PhaseOracle.from_dimacs_file('examples/3sat.dimacs')
oracle.draw()
```

Figure 8 – Command lines and phase oracle circuit in Qiskit

Figure 9 shows a snapshot of the Python code in Qiskit, which runs the oracle and finds the solution of the 3-SAT problem with the Grover’s algorithm.
Figure 9 – Qiskit Python code to run Grover’s algorithm

```python
# Configure backend
backend = Aer.get_backend('aer_simulator')
quantum_instance = QuantumInstance(backend, shots=1024)

# Create a new problem from the phase oracle and the
# verification function
problem = AmplificationProblem(oracle=oracle, is_good_state=v.is_correct)

# Use Grover's algorithm to solve the problem
grover = Grover(quantum_instance=quantum_instance)
result = grover.amplify(problem)
result.top_measurement
```

Figure 5 plots of the solutions obtained with Qiskit.

![Figure 5](image)

Figure 10 – 3-SAT solutions obtained with Grover’s algorithm in Qiskit

Performance of HNN was evaluated with precision, recall, and $F_1$ score, defined as

\[
\text{Precision} = \frac{tp}{tp + fp} \quad (3)
\]

\[
\text{Recall} = \frac{tp}{tp + fn} \quad (4)
\]

\[
F_1 = 2 \times \frac{\text{precision} \times \text{recall}}{\text{precision} + \text{recall}} \quad (5)
\]
Here $t_p$ is true positives, $f_p$ is false positives, and $f_n$ is false negatives. For the dataset containing 4265 one-second spectra, which includes anomaly segment consisting of 95 one-second spectra of $^{137}$Cs source, we obtain $t_p = 100\%$, $f_n = 40\%$, and $F_1 = 75\%$. The $F_1$ score is lower that of 89% obtained for the same data set using conventional implementation of HNN. The run time was 0.057s on the MacOS Monterey with 1.4 GHz processor, and 8GB RAM. For the same data set, the runtime of conventional HNN was 5.1s, so that two orders of magnitude improvement was obtained. Note that for $N = 4625$, $\sqrt{N} = 68$, which is consistent with the observed two orders of magnitude speedup.
5. Conclusions

Environmental screening of gamma radiation consists of detecting weak nuisance and anomaly signal in the presence of strong and highly varying background. In recent prior work, we have developed a Hopfield Neural Network (HNN) in conjunction with an image processing algorithm to detect a weak signal anomaly hidden among the highly fluctuating background spectra. In this report, we investigate the use of quantum computing methods to increase the runtime of HNN. The approach to HNN solution consists using a 3-SAT problem formalism with Grover’s search algorithm on a quantum computing simulator. The 3-SAT problem is a special case of a Boolean satisfiability (B-SAT) problem, which determines if there exists an interpretation that satisfies a given Boolean formula. Grover’s search algorithm allows to search for a particular pattern in an unsorted list. In a classical scenario with N items in a dataset, it would take on average of $O(N)$ queries to sort the database. However, utilizing Grover’s search algorithm only takes $O(\sqrt{N})$ queries. Grover’s algorithm finds possible combinations, and the ones that satisfy the 3-SAT equation are solutions of HNN.

For the dataset containing 4265 one-second spectra, which includes anomaly segment consisting of 95 one-second spectra of $^{137}$Cs source, we obtain $F_1 = 75\%$ and 0.057s runtime. Grover’s algorithm was implemented on Qiskit quantum computing simulator. For the same dataset, performance of conventional HNN was $F_1 = 89\%$ and 5.1s runtime. Using Grover’s algorithm, we have obtained two orders of magnitude improvement in the run time. Future work will focus on improving the accuracy of the HNN solution with B-SAT and Grover algorithm. In particular, we will increase the number of variables in the B-SAT problem.
References


