Chapter 1

Seismic Inversion with Quantum Computing

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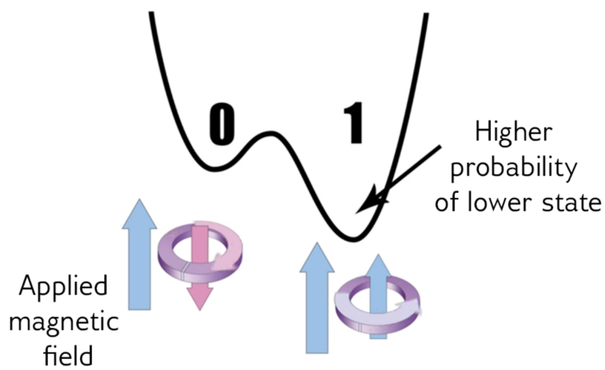

Summary

Project Goals

- Replicate the study conducted by Souza et al. (2022), applying their methodologies and analyses to validate findings and explore implications.
- Provide a comprehensive definition of quantum computers, including an overview of their operational principles and methods for accessing quantum computing resources.
- Execute seismic inversion using quantum computing techniques to illustrate the practical applications and benefits of this technology in geophysical data analysis.
- Discuss potential developments in the field.

Data

The data is based on the data taken from Philippine Sea and available to public (Hodges, 2002).

Introduction

Seismic geophysics relies on complex subsurface modeling derived from numerical analysis of field-collected data. The processing of the vast amounts of data generated in typical seismic experiments can be time-consuming, with significant computational resources needed to create accurate subsurface models. However, in the past decade, quantum computing has seen significant advancements. Quantum computers, which use the principles of quantum mechanics to address computational challenges more quickly than traditional computers, are beginning to demonstrate their potential. The concept of quantum supremacy has been realized with purpose-built quantum machines that can perform specific tasks faster than their classical counterparts. These developments open new opportunities for geoscience and related industries like oil and gas, where quantum computing could offer substantial benefits, enabling faster, more efficient solutions to computationally intense problems.

Quantum annealers have been previously studied for solving systems of linear equations and polynomial equations in. Unlike other quantum algorithms, quantum annealing aims to solve the system $\mathbf{Ax} = \mathbf{b}$ entirely, providing a solution for the vector $\mathbf{x}$. When comparing the performance of quantum annealers with classical computers, we need to consider several factors. These include the cost of preparing the problem, such as mapping the system of linear equations into a Quadratic Unconstrained Binary Optimization (QUBO) or Ising model, the cost of performing the annealing process, and the cost of post-processing the results to derive the solution vector. The velocity inversion problem in geophysics involves determining the distribution of seismic wave velocities in the subsurface by analyzing seismic data. This process is fundamental to seismic imaging and is widely used in oil and gas exploration to understand the geological structures that might contain hydrocarbons.

Quantum Computing in Geophysics

Quantum computers offer several significant advantages. Firstly, they can achieve quantum speed-up, performing certain calculations much faster than classical computers (Shor, 2002). This capability is particularly valuable for complex models where traditional computational methods are both time-consuming and computationally intensive. Furthermore, quantum computers possess unique properties such as superposition, interference, and entanglement (Giana and Eldredge, 2021). Mastering control over these properties could unlock the full potential of quantum computing systems. In terms of optimization, quantum algorithms are capable of physically solving problems, which is a significant leap forward. Additionally, quantum computing holds the promise of overcoming limitations set by Moore's Law (Schaller, 1997), which predicts a plateau in the miniaturization of semiconductor technology. Despite advancements by companies like TSMC or Samsung in developing nano transistors, there is a physical limit to how small transistors can be made before quantum tunneling effects become unavoidable. There are 2 types of quantum computer that we are interested in: gate-based quantum computer and quantum annealer. Their characteristics is depicted in Table 1.1. Our ultimate goal of using quantum computer is to solve 3D elastic FWI by leveraging the advanced computational power of quantum computing. This approach aims to overcome the limitations of classical computing systems. Therefore, are focusing on the optimization problem in quantum annealer.

	Gate-based Quantum Computer	**Quantum Annealer**
Approach	Analogous to classical digital computers, using quantum logic gates to manipulate qubits	Focuses on optimization problems, uses quantum tunneling to find the global minimum of an energy landscape
Applications	Uses quantum logic gates for universal quantum computation, supporting a wide range of quantum algorithms	Specialized in solving specific optimization problems by minimizing an energy function
System	IBM Quantum Experience, Google's Sycamore	D-wave systems
Largest number of qubits	Atom with 1125 qubits, IBM Condor with 1121 qubits	D-Wave's Advantage systems feature 5000+ qubits, have been used for business

Table 1.1: Comparison of Gate-based Quantum Computers and Quantum Annealers. The data is taken from Google, IBM and D-wave websites

Recent studies in Geoscience have employed quantum annealers for hydrology inversion problems (O'Malley, 2018; Golden and O'Malley, 2021). These studies demonstrate that while the size of problems addressable by third-generation D-Wave quantum annealers is small by modern computing standards, they surpass the capacity of Intel's third and fourth generation chips used in similar contexts. Moreover, optimization techniques are essential for seismic inversions, where classical algorithms often become trapped in local minima. Earlier research has suggested that quantum annealing may offer benefits in addressing seismic issues (Alulaiw and Sen, 2015; wei, 2006; Greer and O'Malley, 2020). However, the broader potential of quantum computing in Geoscience remains underexplored in specialized literature. In this work, we are trying to replicate the paper from Souza et al. (2022) by using the D-wave quantum annealer located in British Columbia, Canada. However, the plan we are using is the trial plan, so the usage is limited.

Quantum Annealing

Quantum annealing is a quantum computing technique used to find the global minimum of a given objective function over a given set of candidate solutions. It is particularly useful for solving optimization problems and is based on the principles of quantum mechanics. The process involves setting up the problem as an energy landscape, where each potential solution corresponds to a state with a certain energy. Quantum annealing works by initially superposing the quantum states, allowing the system to explore many possible solutions simultaneously. The system then gradually transitions from a quantum superposition to a classical state through a process called annealing. During annealing, the system is slowly cooled, or the quantum parameters are adjusted, which encourages the system to settle into its lowest energy state—the global minimum of the objective function. This state represents the optimal solution to the problem

At the end of the quantum annealing process, each qubit transitions from a superposition state into a classical state, represented as either 0 or 1 (see Figure 1.1). Initially, the energy diagram during quantum annealing features a single valley, indicative of a superposition state with one minimum. As the process progresses, the energy barrier is elevated, transforming the diagram into a double-well potential. In this configuration, the left valley's low point represents the 0 state, while the right valley's low point corresponds to the 1 state. The qubit will settle into one of these valleys, each with an equal probability of 50%, by the end of the annealing. Additionally, applying an external magnetic field or bias in the same direction as the qubit can skew the double-well potential, increasing the likelihood of the qubit ending in the 1 state. Through manipulation of the bias, control over the energy landscape is achieved, directly influencing the objective function the system aims to optimize.

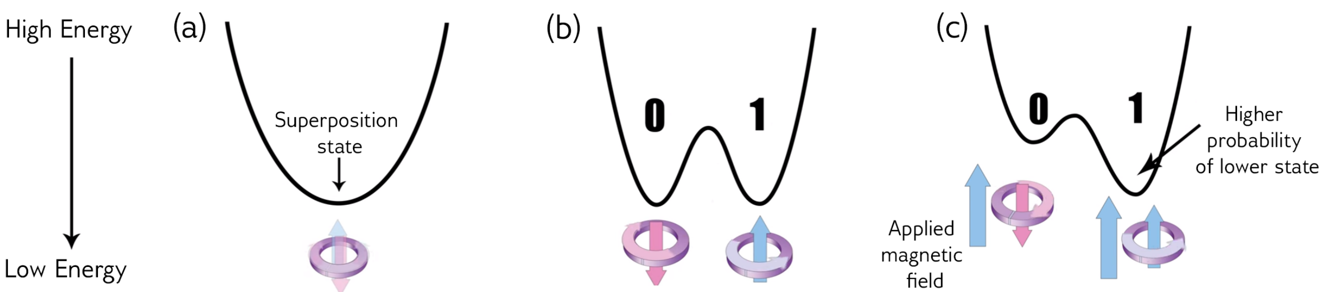

Figure 1.1: Energy diagram changes over time as the quantum annealing process runs and a bias is applied. Figure is captured from D-wave.

Before delving into the various algorithms, it is imperative to comprehend the foundational principles to establish some context. For more details, we suggest to read the paper from Rogers and Singleton (2020). The general problem starts with a graph $G = (V, E)$, where V is the set of vertices and E is the edge set. The QUBO (Quadratic Unconstrained Binary Optimization) Hamiltonian H_G is defined as follows:

$$H_G[Q] = \sum_{r \in V} A_r Q_r + \sum_{r,s \in E} B_{rs} Q_r Q_s \tag{1.1}$$

Here, $Q_r \in \{0, 1\}$ for all $r \in V$. The coefficient A_r is known as the weight at vertex r, while B_{rs} is referred to as the strength between vertices r and s. It might be beneficial to consider (1.1) as the objective function rather than the Hamiltonian, as H_G is a real-valued function and not an operator on a Hilbert space. However, it can easily be mapped to an equivalent Hilbert space form.

$$H_G = \sum_{r \in V} A_r \hat{Q}_r + \sum_{r,s \in E} B_{rs} \hat{Q}_r \hat{Q}_s \tag{1.2}$$

where $\hat{Q}_r = Q_r|Q\rangle$ for all $r \in V$, and I and Q represent the identity and states in the Hilbert space H respectively. The hat denotes an operator on the Hilbert space, and $\hat{Q}_r$ is the corresponding eigenvalue of Q_r with eigenstate $|Q\rangle$. Thus, we can express:

$$H_G|Q\rangle = H_G|Q||Q\rangle \tag{1.3}$$

In this context, terms "Hamiltonian" and "objective function" are used interchangeably. By the QUBO problem, we refer to the problem expressed by the Hamiltonian H_G. The purpose of minimizing the Hamiltonian H_G described in equation (1.2) corresponds to solving the minimization problem stated in equation (1.1) with respect to Q. The Ising model is a prime example of a QUBO problem and is one of the most extensively studied systems in statistical physics. The Ising model consists of a square lattice of spin-1/2 particles with nearest neighbor spin-spin interactions between sites r and s, and when the system is placed in a nonuniform magnetic field, it introduces coupling terms at individual sites r, thereby producing a Hamiltonian of the form:

$$H_G[I] = \sum_{r \in V} B_r E_r I + \sum_{r,s \in E} J_{rs} E_r E_s \tag{1.4}$$

where $E_r = \pm 1/2$. The Ising problem is directly related to the QUBO problem by setting $E_r = Q_r - 1/2$.

Velocity Model

To conduct linear least square inversion using a quantum annealer, we utilize a simplified velocity model derived from data collected in the Philippines Sea (Hodges, 2002). This model consists of 54 stratified layers, each characterized by a constant velocity (see Figure 1.2). The data acquisition process, illustrated in Figure 1.3, assumes a basic scenario where seismic waves generated by the first shot are reflected at the first horizon and received by the first receiver, with similar processes for subsequent shots, receivers, and horizons as depicted in Figure 3. The primary data output from this setup is the two-way travel time, denoted as $\mathbf{t}$. Traditionally, this problem is approached by solving a system of equations $\mathbf{Ms} = \mathbf{t}$, where $\mathbf{M}$ is an $m \times m$ lower triangular matrix (with m being the number of layers), $\mathbf{s}$ is the slowness vector, and $\mathbf{t}$ is the time interval vector. Figure 1.4 presents the results obtained using the classical method for comparison.

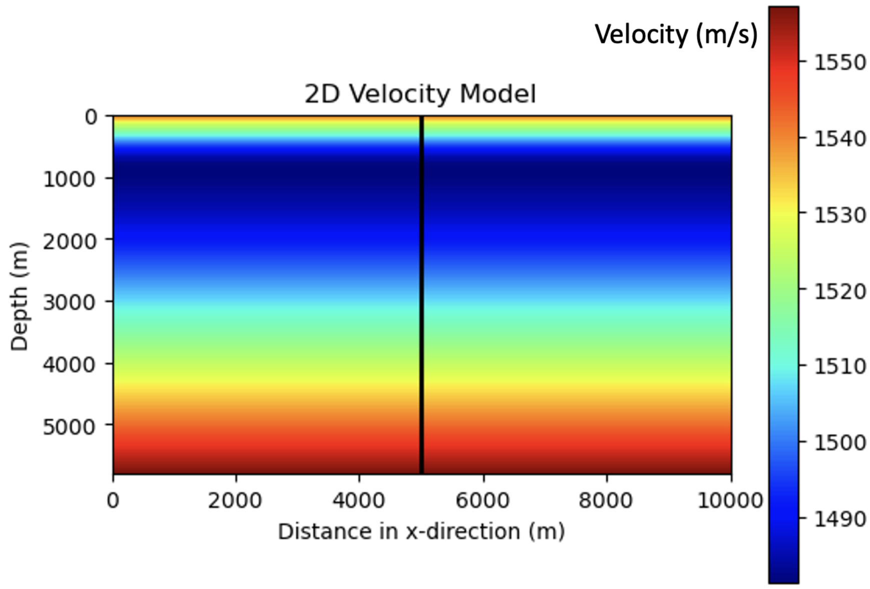

Figure 1.2: Simple velocity model from Philippines Sea

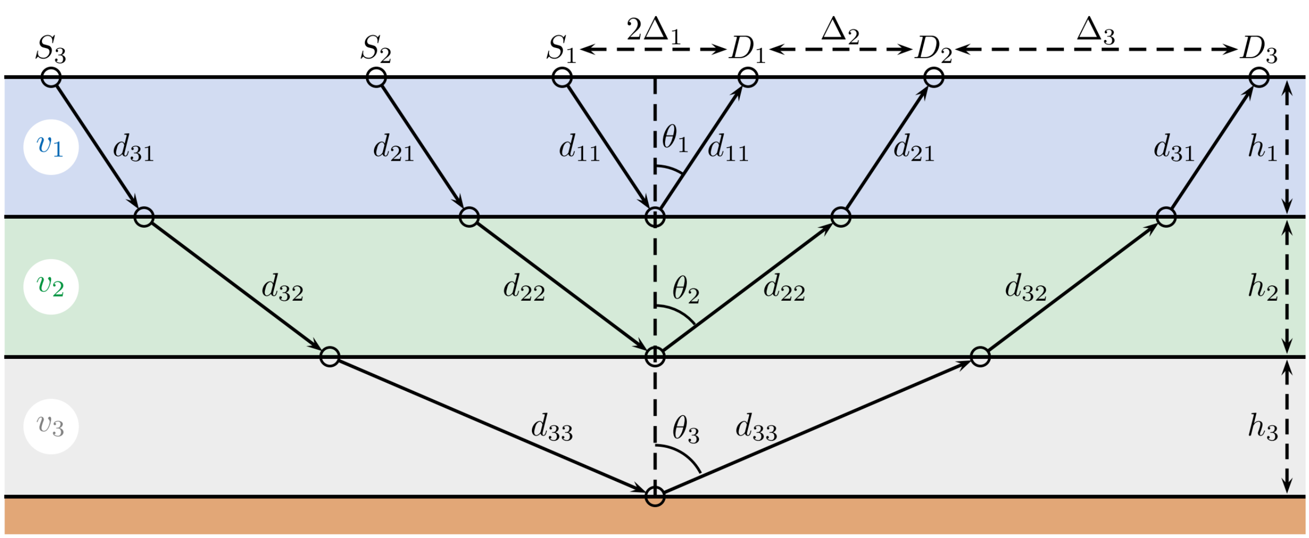

Figure 1.3: Schematics of the siesmic data acquisition

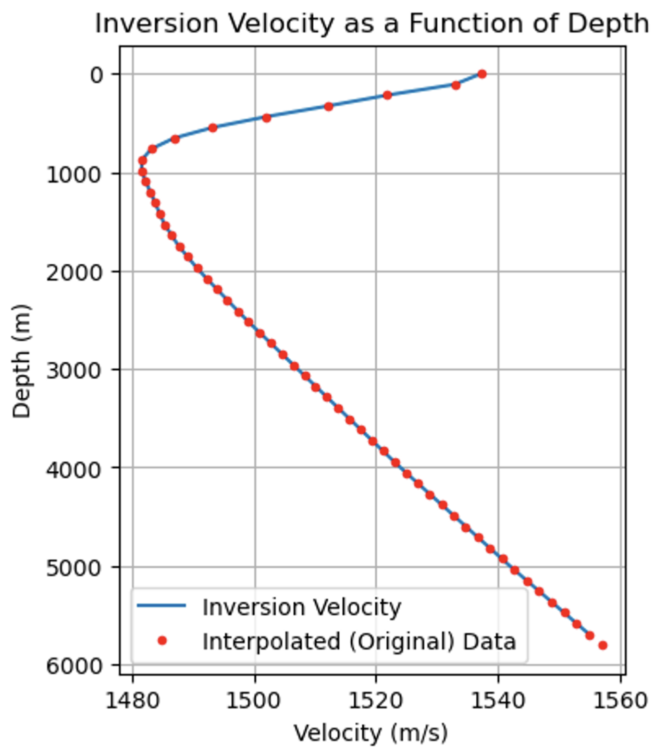

Figure 1.4: Inversion results using classical computer

Linear Least Square Inversion Using the Quantum Annealer

In quantum computers, to solve the system of equations, the problem must first be translated into the QUBO (Quadratic Unconstrained Binary Optimization) formulation. This begins by rewriting the problem from $\|\mathbf{Ms} - \mathbf{t}\|^2$ to $\|\mathbf{Mx} - \mathbf{b}\|^2$, where $\mathbf{s} = \mathbf{s_0} + L(\mathbf{x} - \mathbf{I})$, $0 \leq x_i < 2$, $\mathbf{I}$ is an identity vector, $\mathbf{s_0}$ is the initial guess for s, and L is the boundary limit. Consequently, the new objective function becomes $\|\mathbf{Mx} - \mathbf{b}\|^2$ with $\mathbf{b} = \frac{\mathbf{t} + L\mathbf{MI} - \mathbf{Ms_0}}{L}$.

To accommodate quantum computing constraints, the vector x must be translated into a binary format using an R-bit approximation [cite]. The R-bits approximation involves representing real (floating-point) numbers with a finite number of binary bits as follows:

$$x_i = \sum_{r=0}^{R-1} q_{i,r} 2^{-r}$$

However, translating the problem into the R-bits approximation increases the size of the problem by a factor of R. To address this, a recursive approach, as depicted in Figure 1.5, is employed to improve the precision of floating-point division (Rogers and Singleton, 2020). In the algorithm, only 3 bits were used.

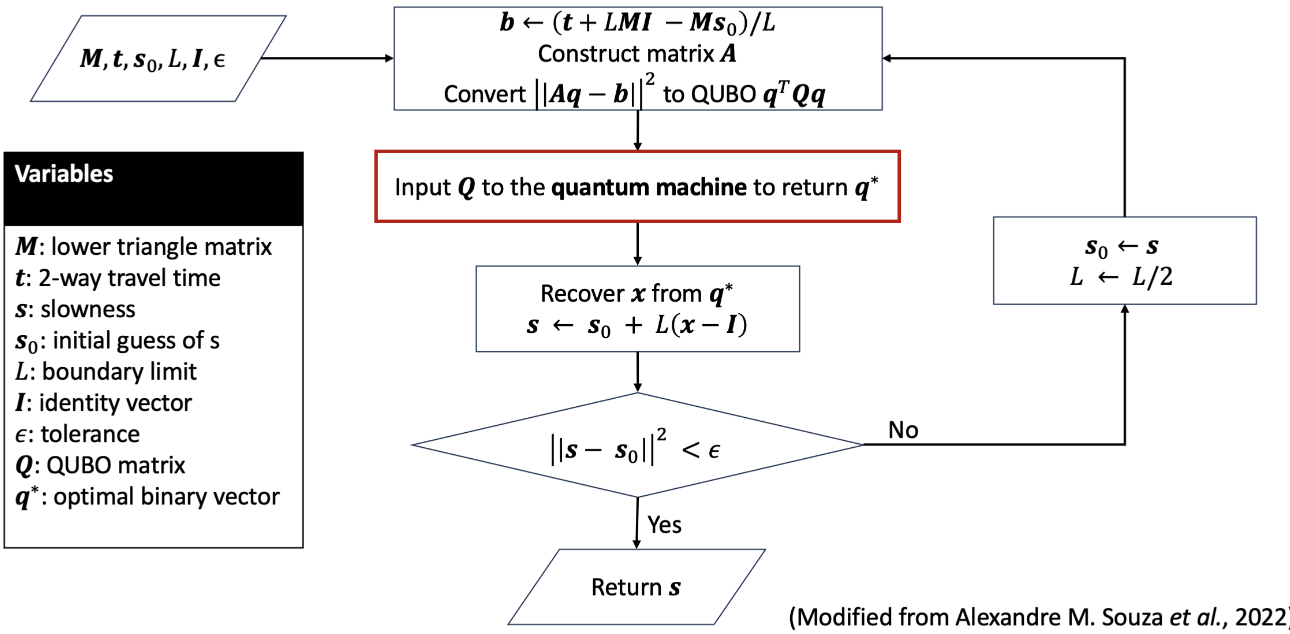

Figure 1.5: Recursive algorithm

Results and Discussion

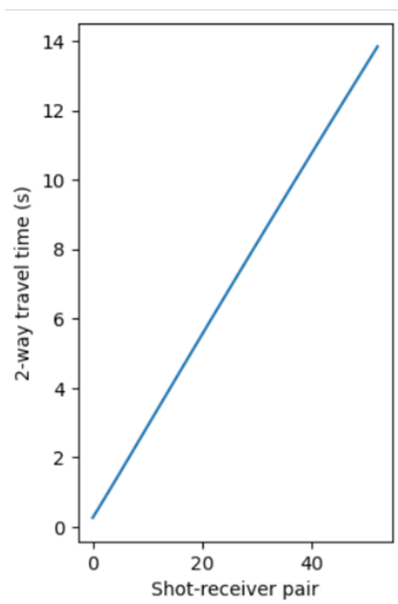

Figure 1.6: The input as 2-way travel time

In this study, we employ a quantum annealer to perform inversion on seismic data, with the input being the 2-way travel time (Figure 1.6). The inversion results (see Figure 1.7), documented over 10 iterations, are graphically represented with three distinct lines: the green line as the initial velocity guess, the blue line as the inversion velocity, and the red line reflecting the original data. As depicted in the results, the blue line progressively moves closer to the red line with each iteration. This convergence suggests that the inversion process is successfully refining the inversion velocity to align more closely with the original data, thereby demonstrating the effectiveness of using quantum annealing in geophysical data inversion. This method not only enhances the accuracy of the inversion results but also indicates potential for significant improvements in computational efficiency and solution precision in seismic data processing.

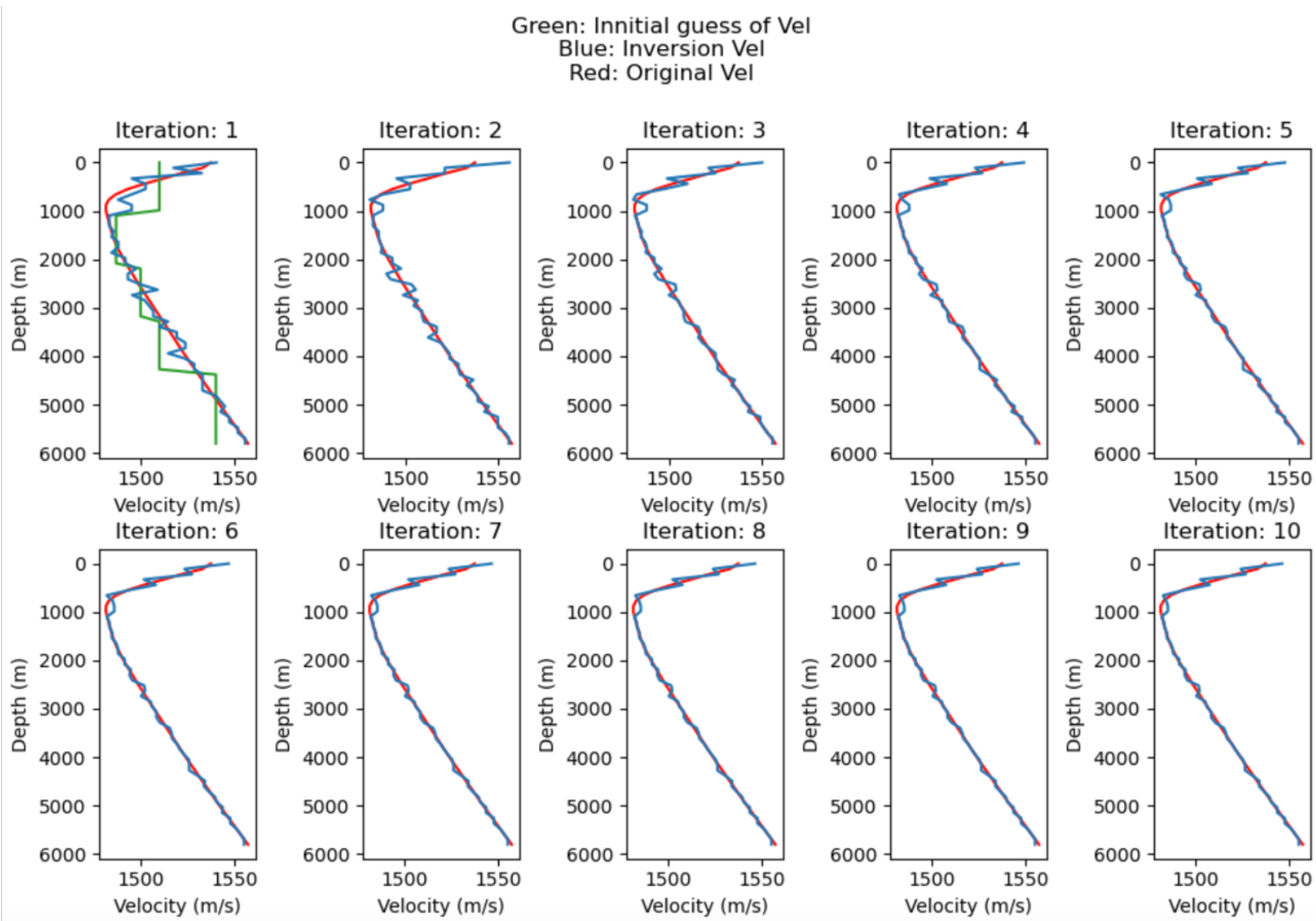

Figure 1.7: Inversion results using quantum computer

Conclusion

In this comprehensive study, we initially translated the given geophysical problem into a QUBO formulation. This crucial step allowed us to leverage the computational capabilities of a real D-Wave quantum computer, facilitating the execution of a linear least square inversion problem. We applied this methodology specifically to field data derived from the Philippine Sea, aiming to demonstrate the practical applicability of quantum computing in real-world geophysical scenarios. Despite achieving successful results, we encountered limitations due to the current developmental stage of quantum hardware, which restricts the size of inversion problems that can be processed effectively. As of now, only smaller-sized datasets can be handled by the existing quantum computational infrastructure. This limitation underscores the nascent nature of quantum computing in handling extensive and complex geophysical data. Looking to the future, our research agenda includes several ambitious objectives aimed at expanding the scope and depth of quantum computing applications in geophysics. We plan to start by performing a simple FWI using our current quantum setup to establish a baseline for what is achievable. Following this, we intend to progressively tackle more complex FWI tasks, which are expected to present greater computational challenges and require more sophisticated quantum algorithms. Additionally, we aim to explore the capabilities of general gate-based quantum computers for performing these inversions. Gate-based quantum computing offers a different paradigm compared to the quantum annealing approach used in D-Wave systems, potentially providing enhanced flexibility and power for solving complex inversion problems. Through these efforts, we hope to significantly advance the integration of quantum computing technology in geophysical data analysis. By pushing the boundaries of what quantum computers can achieve, we anticipate contributing to a deeper understanding of Earth's subsurface structures, ultimately enhancing our ability to interpret geophysical data with unprecedented precision and efficiency.

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