Snell Tomography Using Quantum Annealing

(SEP Report 172, Pages 377 – 396)

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Agenda

Quantum Computing

Snell Tomography Experiment

Algorithms and Results

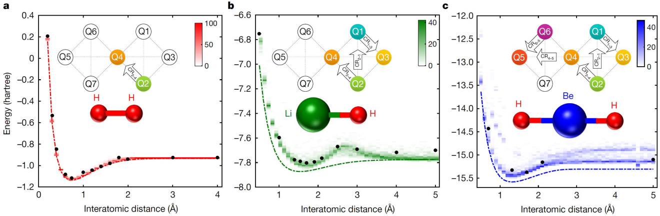
Conclusions

Quantum Computing – Next Bleeding Edge

Problems that are out of reach of conventional computing technology.

Hard problems:

- Large combinatoric optimization problems
- Quantum chemistry & material design
- Quantum cryptography
- Financial services
- Quantum machine learning



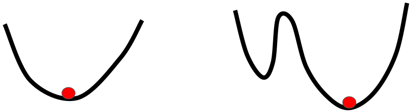
Kandala et al., Nature 549 (2017)

Veni Vidi Vici

- We had an opportunity to run on a quantum computer.
- We came up with a novel combinatoric tomographic challenge.
- We ran on a D-Wave 2000Q quantum annealer.

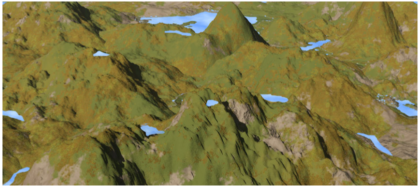
D-WAVE 2000Q Quantum Annealer

- Specialized quantum device
- Finds global minimum for a class of non-convex functions



$$H_t = (1 - \tfrac{t}{T})H_i + \tfrac{t}{T}H_f$$

Adiabatic quantum computing: If you change slowly the initial Hamiltonian to the final Hamiltonian, the system will remain in its lowest energy state.



www.dwavesys.com/quantum-computing

Quadratic Unconstrained Binary Optimization (QUBO)

A quantum annealer (as of today) is best suited to solve the following optimization problem :

Model QUBO Problem

$$
\begin{aligned}
\text{minimize} \quad & x^T Q\, x \\
\text{subject to} \quad & x \in \{0,1\}^n \\
& Ax \leq b \\
& x^T S\, x = d
\end{aligned}
$$

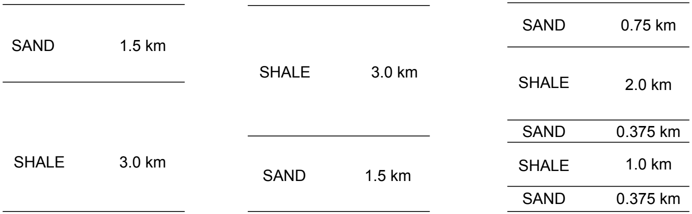
1D Earth Model

- Horizontal layers of unknown thicknesses but known material properties
- The receivers are placed on the top of the layers
- There is one source at the bottom of the layers
- We measure both **travel time** and **offset** for every source-receiver pair

The Simplest Possible Case

1 Ray, 2 Materials

- Sand – 3.0 km/s
- Shale – 2.5 km/s
- Experiment vertical ray
  - Source-receiver distance = 4.5 km
  - Source-receiver traveltime = 1.7 s



Many answers; One sand-shale ratio (1:2)

Question: *Can we determine the fraction of each material in the macrolayer between the source and receivers?*

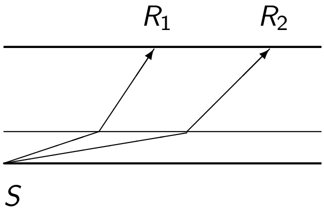


Fig: Experiment Geometry

Parameterization

Horizontal constant thickness layers : We will assume that we have a finite number N of horizontal sublayers with same thickness δ. So total thickness is $N\delta$.

Finite material set : There are only a finite number of materials M, with **fixed known velocities** given by $v_1, \ldots, v_M$.

Finite number of rays : We have a finite number of rays with corresponding travel time measurements are given by $T_1, \ldots, T_K$, and the offsets are given by $L_1, \ldots, L_K$.

Introduce Binary Variables

Introduce binary variables :

$$x_{ij} = \begin{cases} 1 & \text{if sublayer } i \text{ is material } j \\ 0 & \text{otherwise,} \end{cases}$$

for all $i = 1, \ldots, N$ and $j = 1, \ldots, M$.

Introduce constraints :

To ensure that each sublayer gets assigned to one and only one material we will additionally need the family of constraints

$$\sum_{j=1}^{M} x_{ij} = 1 \ , \quad \text{for all } i = 1, \ldots, N.$$

Setup Objective Function

Least Squares Objective Function for k^{th} Ray

$$J_k = \frac{1}{v_{\max}^2}\left(L_k - \sum_{i=1}^{N}\sum_{j=1}^{M}\alpha_{kj}x_{ij}\right)^2 + \left(T_k - \sum_{i=1}^{N}\sum_{j=1}^{M}\beta_{kj}x_{ij}\right)^2$$

Assuming that the k^{th} ray has ray-parameter p_k, we have defined:

- α_{kj} : Horizontal distance traveled by k^{th} ray with ray-parameter p_k in a layer with velocity v_j.
- β_{kj} : Time spent by k^{th} ray with ray-parameter p_k in a layer with velocity v_j.

An Optimization Problem With a Lot of Binary Variables

Leads to a non-convex **"mixed integer program"** :

Sum of Squares Optimization Problem

$$
\begin{aligned}
\text{minimize} \quad & \sum_{k=1}^{K} J_k \\
\text{subject to} \quad & x_{ij} \in \{0,1\}\ ,\ \ \forall\, i \in \{1,\ldots,N\},\ \ \forall\, j \in \{1,\ldots,M\}, \\
& \sum_{j=1}^{M} x_{ij} = 1\ ,\ \ \forall\, i \in \{1,\ldots,N\}.
\end{aligned}
$$

- Continuous variables : The ray-parameters $p_1, \ldots, p_K$
- Binary variables : Layer assignments $x_{11}, \ldots, x_{NM}$
- These are typically hard problems

Alternating Minimization

Continuous Optimization Problem:

- Hold x_{ij}'s fixed, and minimize over p_k's
- Trivial ray tracing

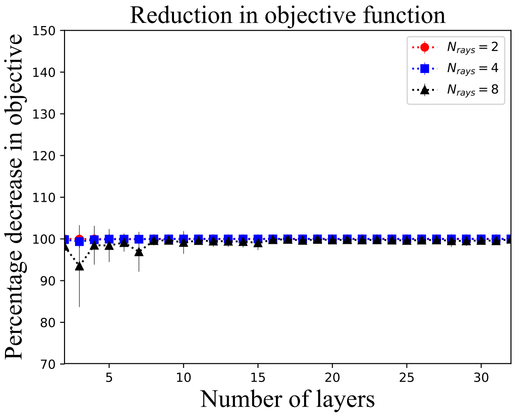
Discrete Optimization Problem:

- Hold p_k's fixed, and minimize over x_{ij}'s
- Combinatorial challenge

Classical Computer Trials

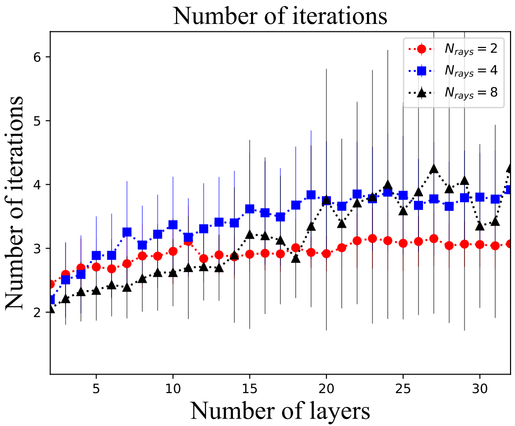
- Take total vertical thickness of 1 km.
- Number of materials $M = 3$.
- Materials :
  - Sandstone – 3.0 km / s
  - Shale – 2.5 km / s
  - Salt – 4.6 km / s
- Number of sublayers was varied from $N = 2, \ldots, 32$.
- Number of rays was varied from $K = 2, 4, 8$.
- For each combination of N and K, 50 independent problem instances were created. For each instance, uniformly spaced p_k's were used to generate the "true" data.
- Each instance was solved 50 times and statistics were gathered.

Classical Results: Reduction In Objective Function



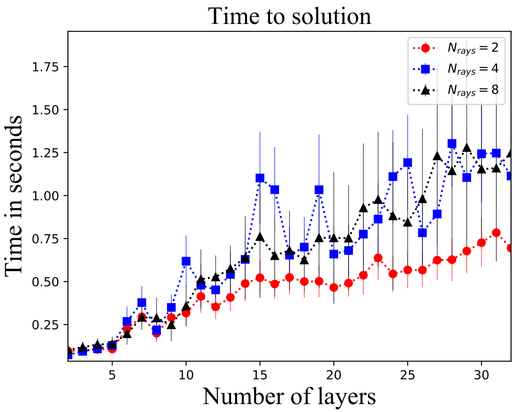
Pretty good reduction in objective function.

Classical Results: Number of Iterations to Converge



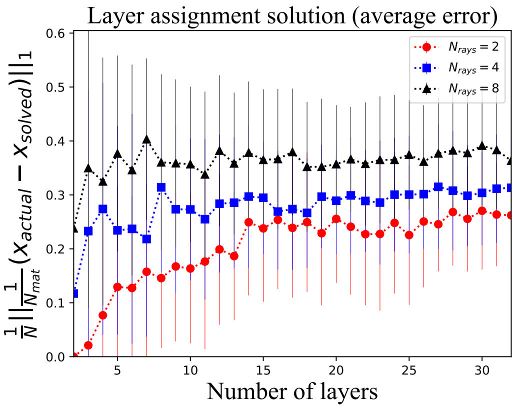
The alternating algorithm converges quite fast in a small number of iterations.

Classical Results: Wall Clock Time to Convergence



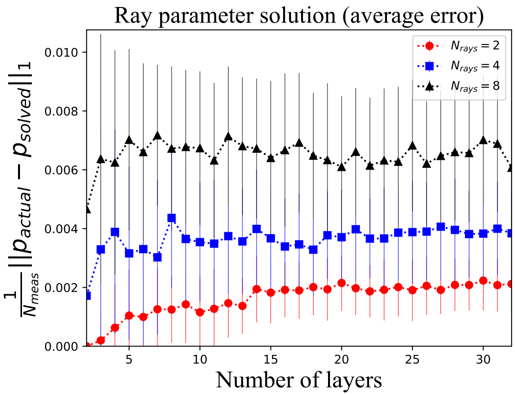
Time to convergence increases with number of layers.

Classical Results: Mean Layer Assignment Error



With the right scaling, errors are constant over number of layers.

Classical Results: Mean Ray-Parameter Error

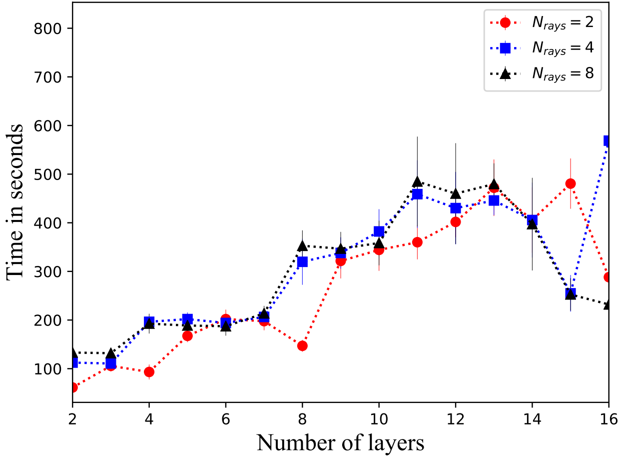


With the right scaling, errors are constant over number of layers.

Preliminary Quantum Solve Trials

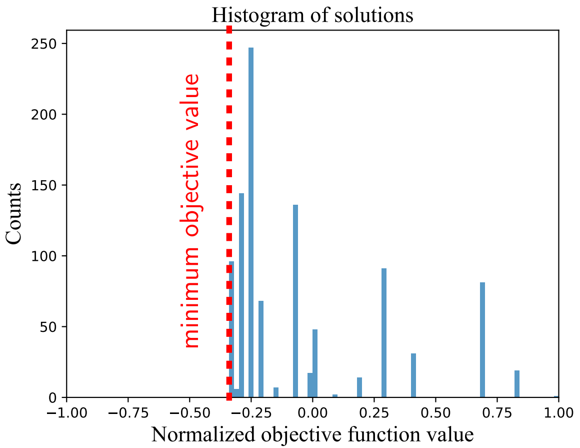
- Same experimental setup as in the classical case.
- We varied $N = 2, \ldots, 16$, and $K = 2, 4, 8$.
- For each combination of N and K, 10 independent problem instances were created. For each instance, uniformly spaced p_k's were used to generate the "true" data.
- We solved each instance of the QUBO problem on the D-WAVE 2000Q quantum annealer 1000 times and gathered statistics on the total time to solution.

Quantum Annealing Results: Time to Solution



The average time per anneal cycle is about same as the time taken to solve the optimization problem on a classical computer.

Quantum Annealing Results: Stochasticity of Annealing



*The quantum annealing process has inbuilt stochasticity. Solutions are recovered close to the lowest energy **“ground state”** of the objective function or Hamiltonian.*

Conclusions

- Solution times were comparable between laptop runs and annealing runs for the small problems.
- For number of binary variables beyond 100, solving the problem through enumeration is nearly impossible for a classical computer.
- This method can also be useful for a kind of *"uncertainty quantification"*, as you can potentially generate an ensemble of solutions that satisfy a given error tolerance.

Future Work

- Sometime after the quantum runs shown in this talk, we obtained a full QUBO formulation. Details in report.
- More accurate benchmarking of the annealing metrics on D-Wave 2000Q.
- Analyze how annealing affects the performance of the alternating optimization algorithm.

Acknowledgments

- We thank Peter L. McMahon for many discussions on quantum computing.
- We thank QC Ware, Corp and D-Wave Systems Inc for giving us permissions to publish the preliminary quantum computing results.

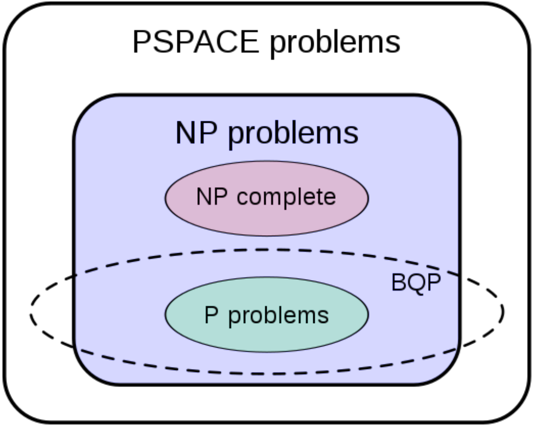
Q & A

Thank You

Questions?

Complexity Diagram

BQP = Bounded-error quantum polynomial time



Problem Structure

- The continuous problem is separable over each ray! So each J_k can be minimized independently.

$$J_k = \frac{1}{v_{\max}^2}\left(L_k - \sum_{i=1}^{N}\sum_{j=1}^{M}\alpha_{kj}x_{ij}\right)^2 + \left(T_k - \sum_{i=1}^{N}\sum_{j=1}^{M}\beta_{kj}x_{ij}\right)^2$$

$$\text{Objective Function :} \quad \sum_{k=1}^{K} J_k$$

- The discrete problem is a *Quadratic Binary Optimization Problem*. Number of binary variables is **NM**.

Question: *Can we reduce the number of binary variables ?*

Towards a Better Combinatorial Optimization Problem: Symmetry of Composition

Symmetry of Composition:

Given an assignment of layers, the objective function is unchanged under arbitrary permutation of layers (this holds because of the horizontal layer assumption). This is a *key observation*.

Key idea: Just count number of times a material repeats. Let y_j denote number of times material j occurs.

- Bound constraint : $0 \leq y_j \leq N$, for all $j = 1, \ldots, M$.
- Sum constraint : $\sum_{j=1}^{M} y_j = N$.

Good but not enough! Only M integer variables, but each variable can take $N + 1$ integer values.

Towards a Better Combinatorial Optimization Problem: Binary Encoding Trick

Binary Encoding Trick:

Since y_j's are positive uniformly spaces integers, work with the binary representation of each variable.

$$y_j = \sum_{l=1}^{r} b_{jl} 2^{l-1} \ , \ \forall \ j = 1, \dots, M \ ,$$

where $r = \lfloor \log_2 N \rfloor + 1$, and $b_{jl} \in \{0, 1\}$.

So now we have $Mr \approx M \log_2 N$ binary variables. This is a $\log \mathbf{N}$ compression.

Equivalent Combinatorial Optimization Problem

Equivalent Optimization Problem

$$\begin{aligned}
\text{minimize} \quad & \sum_{k=1}^{K} \left[\frac{1}{v_{\max}^2} \left(L_k - \sum_{j=1}^{M} \sum_{l=1}^{r} \alpha_{kj} b_{jl} 2^{l-1} \right)^2 \right] + \\
& \sum_{k=1}^{K} \left[\left(T_k - \sum_{j=1}^{M} \sum_{l=1}^{r} \beta_{kj} b_{jl} 2^{l-1} \right)^2 \right] \\
\text{subject to} \quad & b_{jl} \in \{0, 1\} \;,\; \forall\, j \in \{1, \ldots, M\} \;,\; \forall\, l \in \{1, \ldots, r\} \;, \\
& \sum_{j=1}^{M} \sum_{l=1}^{r} b_{jl} 2^{l-1} = N.
\end{aligned}$$

Still a non-convex mixed integer optimization problem.

Alternating Minimization Algorithm

Algorithm 1 Alternating minimization algorithm

procedure ALTERNATING QUBO

// Random assignment
$x_{ij} \leftarrow 0$, for all $i = 1, \ldots, N$ and $j = 1, \ldots, M$
for i = 1 to N **do**
  $j \leftarrow$ Randomly choose from the set $\{1, \ldots, M\}$
  $x_{ij} \leftarrow 1$
Compute $y_j = \sum_{i=1}^{N} x_{ij}$, for all $j = 1, \ldots, M$
Compute b_{jl} as binary representation of y_j, for all $j = 1, \ldots, M$ and $l = 1, \ldots, r$

// Alternating minimization
while Not converged **do**
  $p_k \leftarrow \underset{p_k}{\arg\min}\ J_k$, for all $k = 1, \ldots, K$, and with all b_{jl} fixed.
  $b_{jl} \leftarrow$ solution of QUBO with all p_k fixed.
Compute $y_j = \sum_{l=1}^{r} b_{jl} 2^{l-1}$, for all $j = 1, \ldots, M$

return p_k, y_j for all $k = 1, \ldots, K$ and $j = 1, \ldots, M$

Discrete Search Over Ray-Parameters

Algorithm 2 Global ray parameter search

1: **procedure** DISCRETIZED GLOBAL SEARCH $(k,\ P)$
2: $\quad \Delta p \leftarrow \frac{1}{P\ v_{\max}}$
3: $\quad S \leftarrow \{n\Delta p : n = 0, \ldots, P-1\}$
4: $\quad p_k \leftarrow \underset{p \in S}{\arg\min}\ \frac{1}{v_{\max}^2}\left(L_k - \sum_{j=1}^{M} \frac{\delta p v_j y_j}{\sqrt{1-p^2 v_j^2}}\right)^2 + \left(T_k - \sum_{j=1}^{M} \frac{\delta y_j}{v_j \sqrt{1-p^2 v_j^2}}\right)^2$
5: $\quad$ **return** p_k

P controls level of discretization.

This might seem scary, but is not precisely because ray-parameter search is independent over each ray.

Continuous Search Over Ray-Parameters

Algorithm 3 Newton ray parameter search

1: **procedure** CONTINUOUS LOCAL SEARCH $(k,\ \gamma \in [0,1])$
2: $\quad p_{\min} \leftarrow L_k/(v_{\max}\sqrt{Z^2 + L_k^2})$, $p_{\max} \leftarrow 1/v_{\max}$
3: $\quad p_k \leftarrow \frac{p_{\min}+p_{\max}}{2}$
4: $\quad$ **while** Not converged **do**
5: $\quad\quad p_k \leftarrow p_k - \frac{((1-\gamma)(T(p_k)-T_k)^2+\gamma(L(p_k)-L_k)^2/v_{\max}^2)'}{((1-\gamma)(T(p_k)-T_k)^2+\gamma(L(p_k)-L_k)^2/v_{\max}^2)''}$
6: $\quad\quad p_k \leftarrow \max(p_{\min}, \min(p_{\max}, p_k))$
7: $\quad$ **return** p_k

$\gamma \in [0,1]$ controls how travel time and offset terms are weighed in the search process.

Quantum Annealing Results: Logical Variables vs Qubits