An Introduction to Quantum Computing for Statisticians: Quantum Annealing and More

STAT 853 Final Project

Nikola Surjanovic

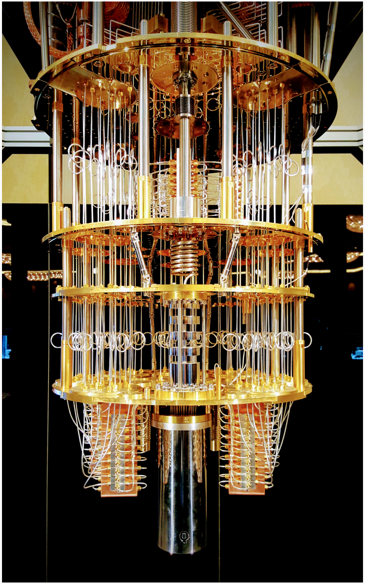
Simon Fraser University

Outline

1. Introduction to Quantum Computers / Applications
2. Quantum Annealing in Statistics
3. Live Demo

Free Access to a Quantum Computer

By the end of today, you will all be able to obtain **free** (limited) access to a quantum computer!



Introduction to Quantum Computers / Applications

According to IBM...

"In five years, the effects of quantum computing will reach beyond the research lab. It will be used extensively by new categories of professionals and developers looking to this emerging method of computing to solve problems once considered unsolvable."[1]

[1] https://www.research.ibm.com/5-in-5/quantum-computing/

Exciting Applications of Quantum Computers

Interesting applications:

- Factoring integers (cryptography)
- Simulating quantum systems
- Computational biology (Li et al., 2018)

What Is a Quantum Computer?

A quantum computer is:

- A device that takes advantage of quantum-mechanical phenomena

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A quantum computer is *not*:

- A replacement for classical computers
- A very, very small computer

Quantum Computer Timeline[2]

Phase 1: Quantum Annealers

We are here

Least powerful, no *known* advantages over classical computers

- Advantages with non-artificial problems hard to find

Applications: Optimization problems

[2] https://www.visualcapitalist.com/three-types-quantum-computers/

Quantum Computer Timeline

Phase 2: Analog Quantum Computers

Could be within the next five years

True quantum speedup

Applications: Material science, quantum chemistry, optimization

Quantum Computer Timeline

Phase 3: Universal Quantum Computers

Might be “exponentially faster” than classical computers

Applications: Machine learning, cryptography, and more

Basic Principles: Quantum Superposition

A *bit* takes on one of two values: 0 or 1

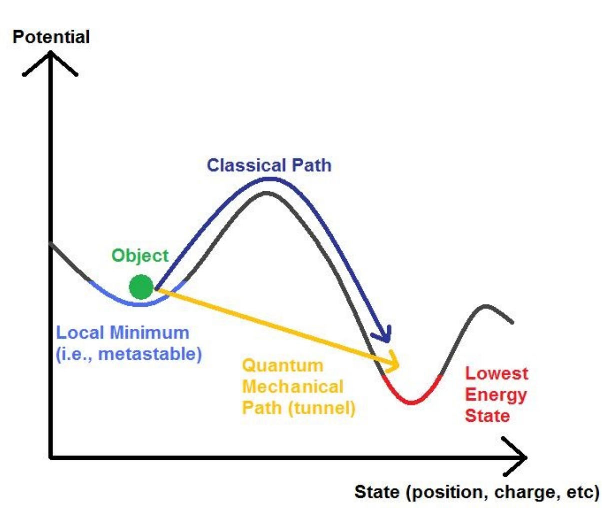
If $|0\rangle$ and $|1\rangle$ are two states, a *qubit* is in a state

$$c_0|0\rangle + c_1|1\rangle,$$

where $c_0, c_1 \in \mathbb{C}, |c_0| + |c_1| = 1$

Once *observed*, $P(\text{qubit} = 0) = |c_0|$, $P(\text{qubit} = 1) = |c_1|$

Basic Principles: Quantum Tunneling



“Cranberry”, https://commons.wikimedia.org/wiki/File:QuantumTunnel.jpg, Public Domain

Basic Principles: Quantum Entanglement

A pair (or group) of quantum particles are “entangled”

- The state of one particle is related to the state of another particle
- Particles might be separated by very large distances!

Einstein: “spooky action at a distance”

Quantum Supremacy

Fall 2019: Google AI and NASA claim “quantum supremacy”

Google’s quantum processor completed a task in 3 minutes and 20 seconds[3]

- Would take the world’s fastest supercomputer 10,000 years
- Disputed claim

[3] https://www.technologyreview.com/f/614416/google-researchers-have-reportedly-achieved-quantum-supremacy/

Quantum Annealing in Statistics

Oleg Alexandrov, https://commons.wikimedia.org/wiki/File:D-wave_computer_inside_of_the_Pleiades_supercomputer.jpg,

The QUBO Model

QUBO: Quadratic Unconstrained Binary Optimization

Find $q_i \in \{0, 1\}$ that minimize

$$\text{Energy} = \sum_i a_i q_i + \sum_{i<j} b_{ij} q_i q_j$$

The QUBO Model

$$\text{Energy} = \sum_i a_i q_i + \sum_{i<j} b_{ij} q_i q_j$$

As a matrix (if $n_q = 3$):

$$K_1 = \begin{bmatrix} a_1 & b_{12} & b_{13} \\ 0 & a_2 & b_{23} \\ 0 & 0 & a_3 \end{bmatrix}$$

The Adiabatic Theorem

Adiabatic theorem: **core idea** behind quantum *annealing*

Suppose we can easily find the q_i that minimize energy for an initial problem, K_0

If we can *slowly* transition to our problem, K_1, the q_i will remain in the lowest-energy state

Find solution to K_0, which is chosen to be easy to solve

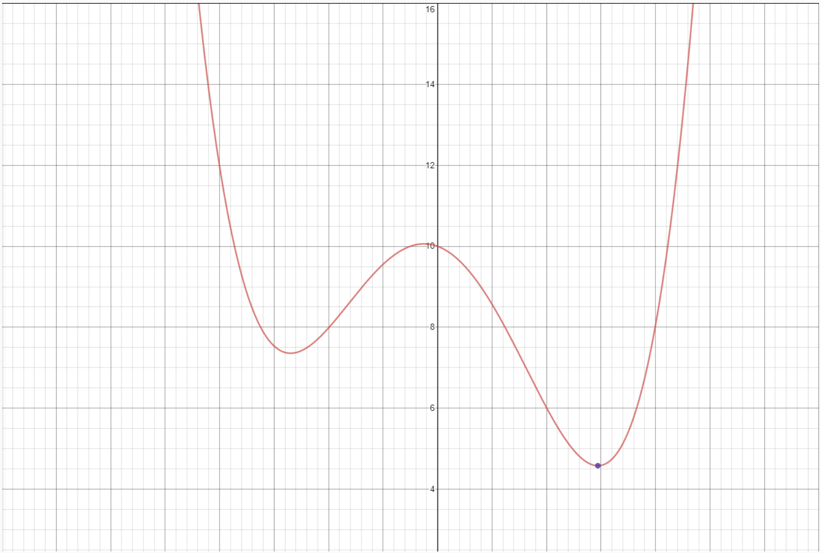
$$K_0 = \begin{bmatrix} a_1^{(0)} & b_{12}^{(0)} & b_{13}^{(0)} \\ 0 & a_2^{(0)} & b_{23}^{(0)} \\ 0 & 0 & a_3^{(0)} \end{bmatrix} \to \begin{bmatrix} a_1^{(1)} & b_{12}^{(1)} & b_{13}^{(1)} \\ 0 & a_2^{(1)} & b_{23}^{(1)} \\ 0 & 0 & a_3^{(1)} \end{bmatrix} = K_1$$

Quantum Annealing

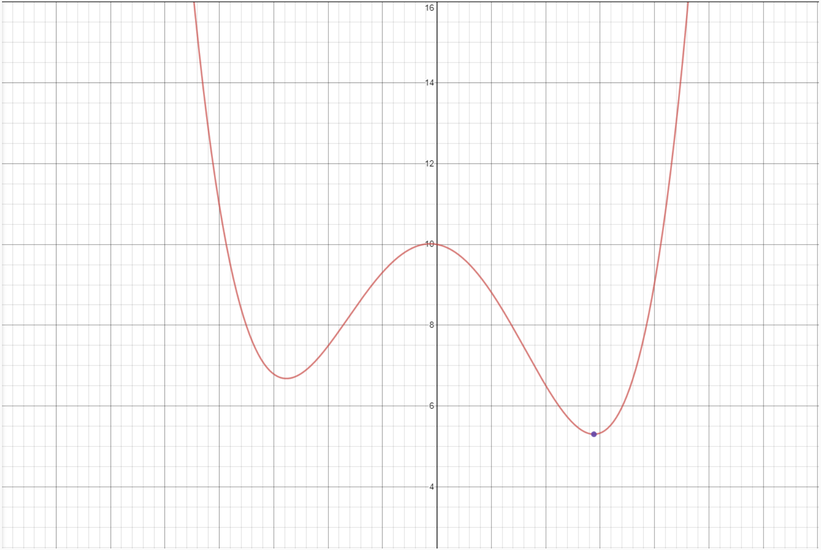
Transition to our problem, K_1

Note

Think of this as slowly changing the “landscape” of peaks and troughs over which we try to find a global minimum



https://www.desmos.com/calculator



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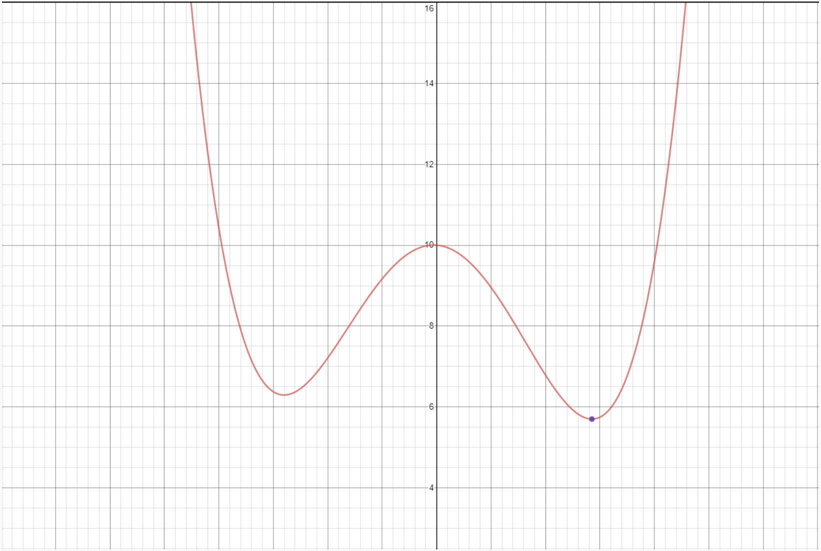


https://www.desmos.com/calculator

Applications

We will discuss three applications of quantum annealing, from Foster et al. (2019), and one from Li et al. (2018)

1. Maximum likelihood estimation
2. Experimental design
3. Inversion of matrices (e.g. for Gaussian process regression)
4. Computational biology

Application 1: Maximum Likelihood Estimation

Very common in statistics

For $X_1, \ldots, X_n \overset{iid}{\sim} f(x|\theta)$, find θ that maximizes

$$\sum_{d=1}^{n} l(\theta|x_d),$$

where $l(\theta|x_d) = \log(f(x_d|\theta))$

Application 1: Maximum Likelihood Estimation

With n_q qubits, express

$$\theta = \sum_{j=1}^{n_q} 2^{p_j} q_j$$

Example: $p_j \in \{-2, -1, 0, 1, 2\}$

Use a second-order Taylor series about some $\theta^{(0)}$ to approximate $l(\theta|\mathbf{x})$ as a quadratic

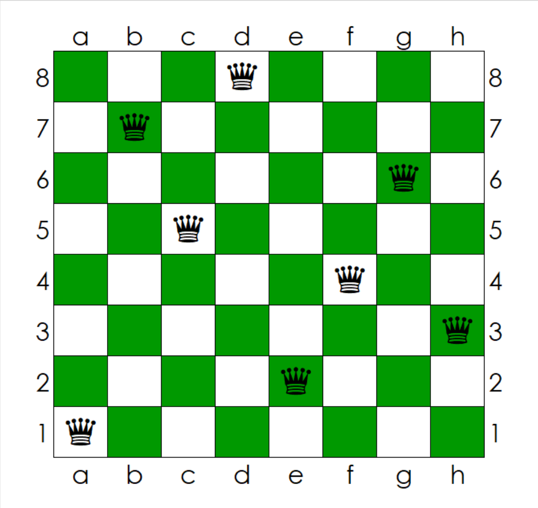
Application 1: Maximum Likelihood Estimation

$$l(\theta|\mathrm{x}) \approx \sum_{i=1}^{n_q} a_i q_i + \sum_{i<j} b_{ij} q_i q_j,$$

for some a_i, b_{ij}

Obtain $\theta^{(1)}$, expand around $\theta^{(1)}$, and repeat

Application 2: Experimental Design



Application 2: Experimental Design

Another application: Finding Latin hypercubes

"Finding an optimal design generally scales exponentially … and quantum annealing may provide a polynomial increase in computational speed for high dimensional problems." (Foster et al., 2019)

Application 2: Experimental Design

Can be placed into QUBO form

- Place a qubit on each cell

Application 2: Experimental Design

$$\text{Energy} = \sum_i a_i q_i + \sum_{i<j} b_{ij} q_i q_j$$

$$a_i = -2$$

$$b_{ij} = \begin{cases} 2, & i, j \text{ in same row or column} \\ 1, & i, j \text{ on same diagonal} \\ 0, & \text{otherwise} \end{cases}$$

Application 3: Inversion of Matrices

Inversion of large matrices occurs in Gaussian process regression

- Can be a major bottleneck

Possible to view matrix inversion as an optimization problem!

Application 4: Computational Biology

Li et al. (2018) ranked transcription factor binding affinities using a quantum annealer and some classical machine learning methods

Found that “quantum annealing might be an effective method to implement machine learning for certain computational biology problems”.

Live Demo

Live Demo Details

Access D-Wave 2000Q quantum computer via D-Wave Leap2

Can use Python (no R interface at the moment)

Example: experimental design

Summary

1. Quantum computers have great potential for use in many fields of science
2. These machines make use of quantum superposition, entanglement, and tunneling
3. Basic quantum *annealers* have arrived and can be used for small problems at the moment

References

Robert C Foster, Brian Weaver, and James Gattiker. Applications of quantum annealing in statistics. *arXiv preprint arXiv:1904.06819*, 2019.

Richard Y Li, Rosa Di Felice, Remo Rohs, and Daniel A Lidar. Quantum annealing versus classical machine learning applied to a simplified computational biology problem. *NPJ quantum information*, 4(1): 1–10, 2018.

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Other Sources

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- https://www.technologyreview.com/f/614416/google-researchers-have-reportedly-achieved-quantum-supremacy/
- https://www.wired.com/2013/10/computers-big-data/

Thank You!

Questions?

Bonus Material

Application 5: Feature Selection

Example: Linear regression, p covariates

- All-subsets selection: 2^p possible choices

Using mutual information of pairs of random variables (somewhat like correlation), can place into QUBO form (to a certain extent)