Numerical Statistics and Quantum Algorithms

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Quantum Computing and Healthcare Statistics

- In partnership with ICON, Lockheed Martin is exploring computational challenges in healthcare that can be addressed at their latest generation D-Wave quantum computer.*

- The research is focused on development and implementation of new algorithms to empower the inferential statistics and predictive data analytics in healthcare.

- The nearest objective is to translate real life statistical problems in drug development into algorithms and codes for D-Wave computer.

* *The D-Wave customers include Lockheed Martin and a consortium including Google and NASA. In January Temporal Defense Systems, a cyber-security firm, bought one. The Economist, March 11-17th, 2017, p.9*

Outline

- Intro
- Quantum algorithms
- D-wave and Ising model
- Problems of interest
- Expectations

From quantum physics to quantum computing

- Actual objects of microphysics
- Elegant mathematical models
- Amazing theoretical results that follow
- Various interpretations of these results
- Building objects that fit those models
- Are they identical or at least similar in behavior to actual objects?
- Imaginary universal quantum computers and respective algorithms
- Evolution of existing quantum machine

An elegance of mathematical physics

- Time-dependent Schrodinger equation (general):

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \hat{H}\Psi(\mathbf{r},t)$$

- Time-dependent Schrodinger equation (single nonrelativistic particle):

$$i\hbar\frac{\partial}{\partial t}\Psi(\mathbf{r},t) = \left[\frac{-\hbar^2}{2\mu}\nabla^2 + V(\mathbf{r},t)\right]\Psi(\mathbf{r},t)$$

- Schrodinger - Belavkin quantum filtering equation:

$$d\Psi = -\left(\frac{1}{2}L^*L + \frac{i}{\hbar}H\right)\Psi dt + L\Psi dy$$

Quantum algorithms

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- Quantum simulations, see QMCPACK: http://qmcpack.org/ https://github.com/QMCPACK/qmcpack/raw/develop/manual/qmcpack_manual.pdf
- Quantum search, ordering, factorization, …
- Quantum machine learning, support vector machine for big data classification
- Quantum Monte-Carlo methods
- Clustering

Note: Many theoretical publications but only toy examples

D-Wave is now shipping its new $15 million, 10-foot tall quantum computer

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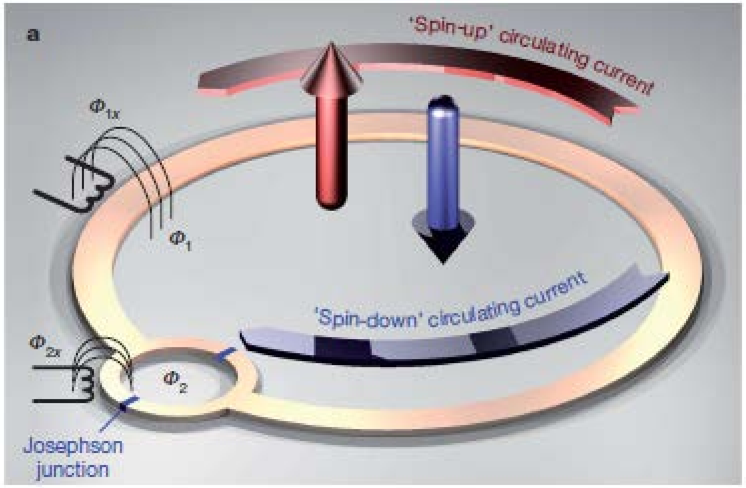
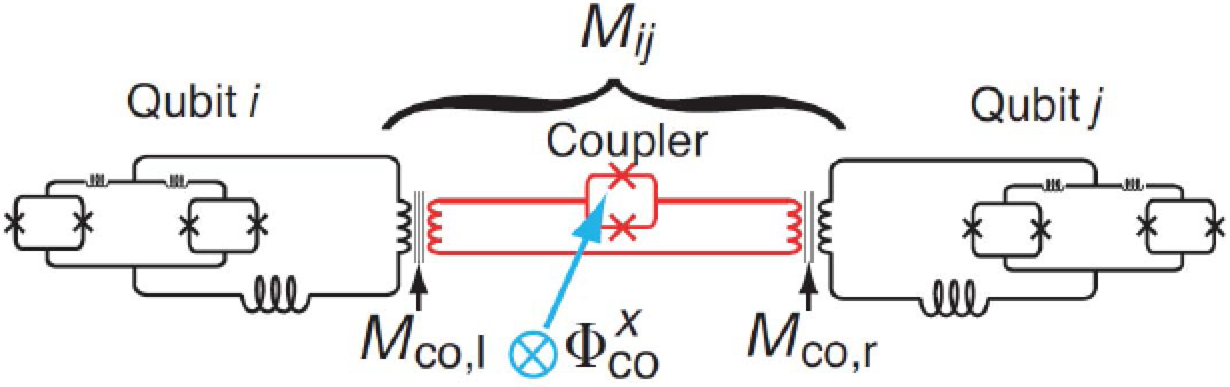
With 2000 qubits and new control features, the new system can solve larger problems than was previously possible, with faster performance, providing a big step toward production applications in optimization, cybersecurity, machine learning, and sampling.

Hardware model





Quantum adiabatic optimization based on Ising model

- Quantum annealing:

$$H(t,T) = (1-\gamma(t,T))H_0 - \gamma(t,T)H_P$$

$$\gamma(t,T) = t/T, \;\; T = O\left[\exp\left(\alpha N^{\beta}\right)\right]$$

$$H_P(\mathbf{x}) = -\mathbf{x}^T\mathbf{D}\mathbf{x} - \mathbf{h}^T\mathbf{x}, \;\; H_0(\mathbf{x}) = \mathbf{h}_0^T\mathbf{x}, \;\; x_i = \mp 1$$

- All solutions are based on analogue quadratic unconstrained binary minimization:

$$\mathbf{x}^* = \operatorname{Arg}\min_{\mathbf{x}} \left[\mathbf{x}^T\mathbf{D}\mathbf{x} + \mathbf{h}^T\mathbf{x}\right]$$

- Ising formulations of many NP problems can be found in papers by A. Lucas (2014) and V. Smelyanskiy et all (2014)

Methods, Algorithms and Applications

Statistics and predictive analytics / Quantum algorithms	Combinatorial and optimal design	Machine learning and classification (SVM, NNets, CA)	Item/subject matching	Stochastic models of clinical trial execution
Quantum annealing (Hamiltonian based optimization)	CCT design with multiple competing treatments/drug combinations	• Genomics, proteomics • Population analytics • Study clustering	Selection of virtual subjects for comparator arms from MDBs	Cost minimization under ethical, resource and regulatory constrains
Quantum Monte-Carlo algorithms	Statistical properties of adaptive designs for PK/PD/DF models			Simulation of complex trials based on mechanistic models
Grove’s search algorithm(s)			• Detection of rare events in MDBs • Selection of quasi-identical subjects	

Example: Design of cluster clinical trials*

- Targeted problem:
  - The number of cancer types -> K
  - The number of drugs -> N, the number of treatments to be screened –> J = N(N-1)/2
  - The number of blocks (medical centers, biomarkers, …) -> L
- Constraints:
  - All blocks involve the same number of cancer types - K_1
  - All blocks use the same number of drugs - N_1
  - Each pair of distinct cancer types are involved together at L_1 medical centers
  - Each pair of distinct drugs are used together at L_2 medical centers
  - Each drug is used on each type of cancer at L_3 medical centers

**The "combinatorial design" component of this research project was launched together with Professors R. Bailey and P. Cameron, University of St. Andrews in 2015, at the workshop on Design and Analysis of Experiments in Healthcare held at the Isaac Newton Institute for Mathematical Sciences, University of Cambridge, UK.*

BIBD that reduces the number of sub-trials from 60 to 30

T1=D1,5 , … , T10=D4,5

Operational and medical constraints:
- No more than 3 cancer types per block
- Only 2 drugs per treatment

	Cancer					
Block	**C1**	**C2**	**C3**	**C4**	**C5**	**C6**
1	D1,5	D1,5	D1,5			
2	D1,2				D1,2	D1,2
3	D2,3		D2,3	D2,3		
4	D3,4	D3,4				D3,4
5	D4,5			D4,5	D4,5	
6		D1,3		D1,3	D1,3	
7		D2,4	D2,4		D2,4	
8			D3,5		D3,5	D3,5
9			D1,4	D1,4		D1,4
10		D2,5		D2,5		D2,5

Properties:
- Every pair of drugs at one trial
- Every pair of cancer types at two trials
- Every drug with every cancer type at two trials

Benchmarking: in reality "practical" designs take into account medical knowledge, disease prevalence, differing enrollment rates per cancer type and competing products

Related design problem

- Model: $\mathbf{Y}_i = \mathbf{\Theta}^T \mathbf{x}_i + \varepsilon_i$
- Candidate set: $\mathbf{x}_i \in \mathfrak{X}_d \subset \mathfrak{X}$
- Optimization problem:

$$\xi_N^* = \operatorname{Arg}\min_{\xi_N} \Psi[\mathbf{M}^{-1}(\xi_N)], \quad \xi_N = \{\mathbf{x}_i\}_1^N$$

or more specifically:

$$\xi_N^* = \operatorname{Arg}\max_{\xi_N} |\mathbf{M}(\xi_N)|$$

$$\mathbf{M}(\xi_N) = \sum_{i=1}^{N} \mathbf{x}_i \mathbf{x}_i^T$$

Note: number of possible designs $C_N^n = \frac{n!}{N!(n-N!)}$

Second order exchange algorithm*

Given $\xi_{N,(s)}$ find $\mathbf{x}_i^{(s)} \in \xi_{N,(s)}$ and $\mathbf{x}^{(s+1)} \in \mathscr{X} \setminus \xi_{N,(s)}$ such that their swapping maximizes the increment of

$$\frac{|\mathbf{M}(\xi_{N,(s+1)})|}{|\mathbf{M}(\xi_{N,(s)})|} = 1 + \Delta_s \quad .$$

One can verify that

$$\Delta_s = \mathbf{x}^T \mathbf{M}^{-1}(\xi_{N,(s)})\mathbf{x} - \mathbf{x}_i^T \mathbf{M}^{-1}(\xi_{N,(s)})\mathbf{x}_i$$

$$+\mathbf{x}^T \mathbf{M}^{-1}(\xi_{N,(s)})\mathbf{x}_i \mathbf{x}_i^T \mathbf{M}^{-1}(\xi_{N,(s)})\mathbf{x} - \mathbf{x}^T \mathbf{M}^{-1}(\xi_{N,(s)})\mathbf{x}\mathbf{x}_i^T \mathbf{M}^{-1}(\xi_{N,(s)})\mathbf{x}_i$$

- N calls of “quantum annealing” is needed at every iteration

**Fedorov V. (1972) Theory of Optimal Experiments. Academic Press*

Key references

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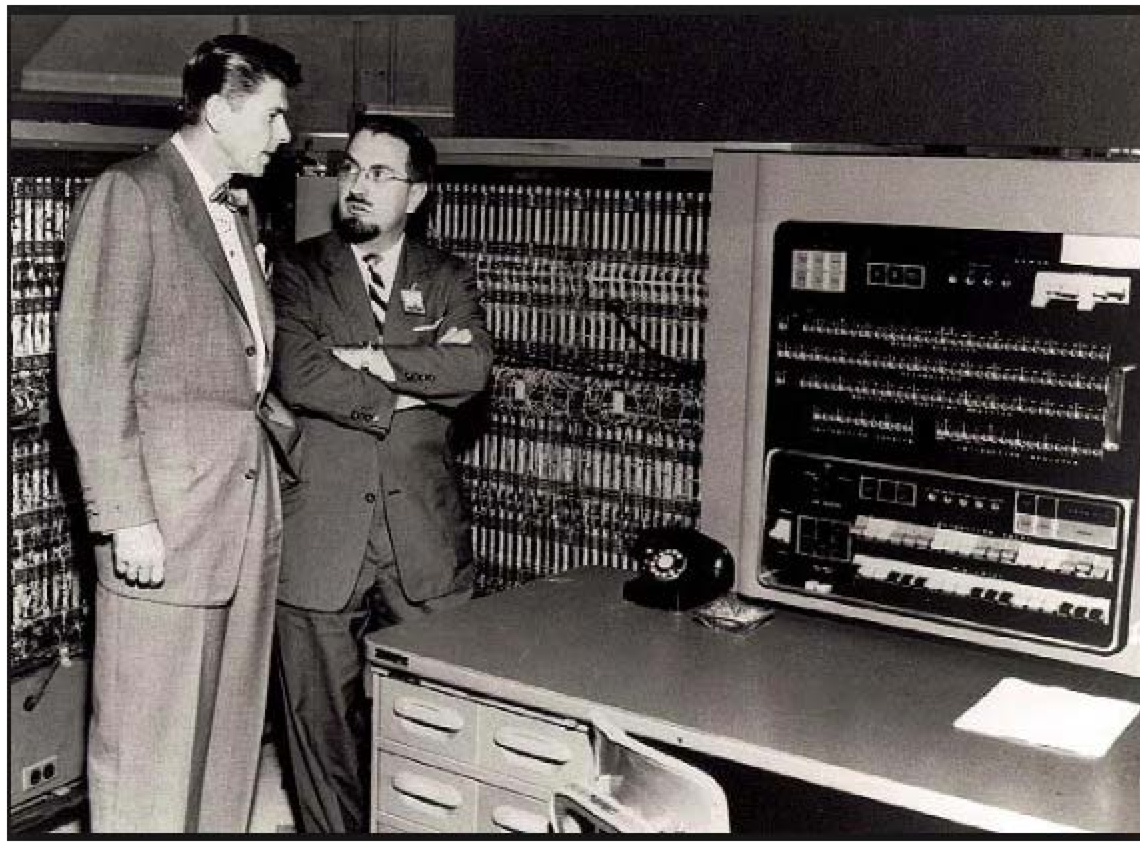
Fixed-purpose electromechanical computer: deciphering the codes of the German Enigma machine used by its armed forces to encrypt its communications. Yes it is "Turing-complete". Its clock speed started being of 0.8 and got to be of 2Hz

https://www.wired.com/2014/11/imitation-game-building-christopher/#slide-2

After 12 years

IBM 701 meets the future president

In 1954, Ronald Reagan, who was a TV personality for General Electric at the time, visited the GE Aircraft Jet Engine Plant in Evendale, Ohio. During this visit, GE manager Herbert Grosch spent a few minutes introducing the future US president to the IBM 701.



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