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ОПЕРАТИВНА ПРОГРАМА
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ИНТЕЛИГЕНТЕН РАСТЕЖ

Using quantum annealers for solving optimization problems: introduction

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ЦЕНТЪР ЗА ВЪРХОВИ ПОСТИЖЕНИЯ ПО
ИНФОРМАТИКА И ИНФОРМАЦИОННИ И
КОМУНИКАЦИОННИ ТЕХНОЛОГИИ

Talk outline

- Models for quantum computing
  - Quantum information
  - Three models for QC
    - Gate model
    - Adiabatic computing
    - Quantum annealing
      - The D-Wave QA
- Solving optimization problems using QA/D-Wave
  - Phases of solving a problem on DW
  - Example 1: Maximum Cut
  - Example 2: Maximum Clique
- Conclusion and Q&A

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Models for quantum computing

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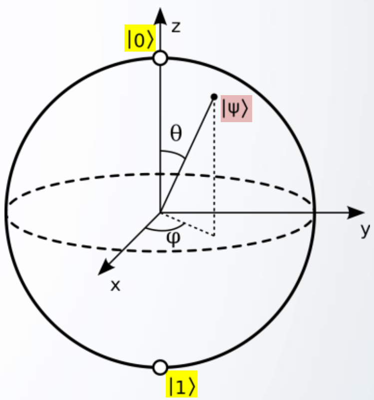
Quantum information

- Quantum vs classical unit of information
  - Classical unit: **bit**, describes a state either 0 or 1
  - Quantum unit: **qubit**: superposition of 0 and 1 ("both 0 and 1")
  - The state of 1 qubit is described using 2 complex numbers:

$$\alpha_0 |0\rangle + \alpha_1 |1\rangle$$
$$(|\alpha_0|^2 + |\alpha_1|^2 = 1)$$

  - **Bloch sphere**: geometric representation of all possible states of a qubit



  - $|\alpha_0|^2$ and $|\alpha_1|^2$ are the probabilities for outcomes $|0\rangle$ and $|1\rangle$ when the qubit is measured

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Quantum information (cont.)

- Classical vs quantum <u>register</u> (*n* units)
  - Classical: *n* bits can describe a number between 0 and 2^{n-1} (the state of a classical register is described by a single number)
  - The state of *n* <u>*entangled*</u> qubits is described by 2^n complex numbers:

$$n = 2: \ |q_2\rangle = \alpha_{00}\,|00\rangle + \alpha_{01}\,|01\rangle + \alpha_{10}\,|10\rangle + \alpha_{11}\,|11\rangle$$

$$= \begin{bmatrix}\alpha_{00} & \alpha_{01} & \alpha_{10} & \alpha_{11}\end{bmatrix}^T \quad 2^2 \text{ numbers}$$

$$n = 3: \ |q_3\rangle = \alpha_{000}\,|000\rangle + \alpha_{001}\,|001\rangle + \cdots + \alpha_{111}\,|111\rangle$$

$$= \begin{bmatrix}\alpha_{000} & \alpha_{001} & \dots & \alpha_{111}\end{bmatrix}^T \quad 2^3 \text{ numbers}$$

$$\dots$$

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The good and the bad about quantum states

- The good
  - *n* entangled qubits may encode $\sim 2^n$ numbers (amplitudes)
  - Even a 1-qubit *gate* may change exponential # of amplitudes
- The bad
  - A measurement ("reading") yields a single basis vector*, e.g.* $|0100\rangle$
  - Decoherence: interactions with outside environment such as temperature fluctuations, electromagnetic waves, and vibrations can destroy quantumness.
  - Programming is inflexible and non-intuitive: no conditionals, no copying and/or saving information (no-cloning theorem).
- What are most popular models for quantum computing?

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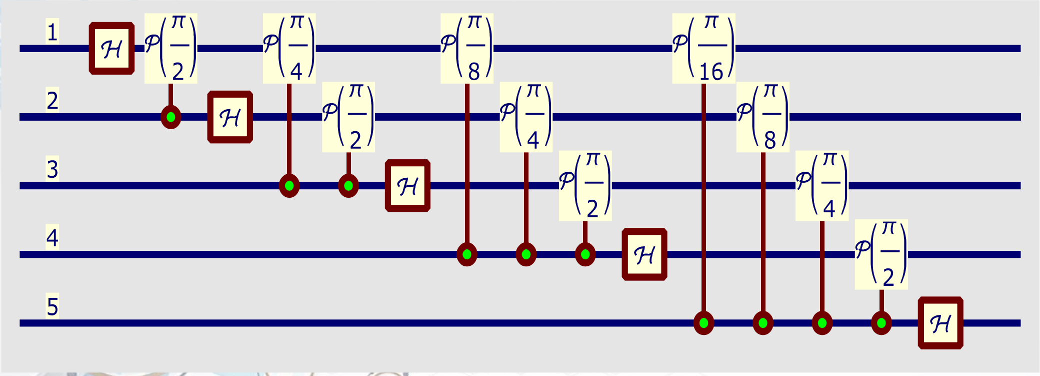
Universal (gate model) quantum computers

- Gate model of quantum computing
  - Sequence of transformation (gates) on quantum registers



Quantum Fourier Transform

  - Polynomial algorithm for integer factorization (Shor 1994)
  - Holds longer-term promise
  - Currently: largest computers with only 50-60 qubits.

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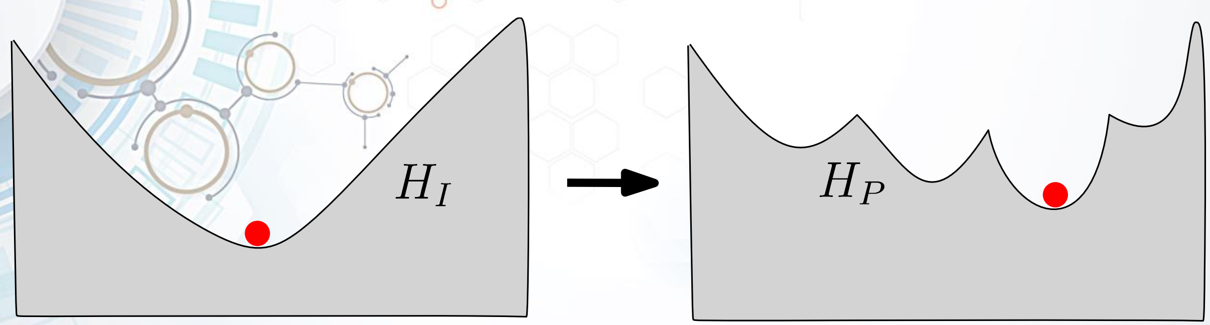
Adiabatic quantum computing

- Based on the fact that quantum systems tend to stay in a minimum-energy state
- Adiabatic theorem: a quantum system will stay in its ground (minimum energy) state if the Hamiltonian describing the system is changed “sufficiently slowly” (adiabatically)



$$H(s) = (1 - s)H_I + s\, H_P$$

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Adiabatic quantum computing (cont.)

- To find a solution to an optimization problem:
  - Construct problem Hamiltonian H_P whose ground state encodes the solution of our problem *P*;
  - Initialize quantum system in a ground state of a Hamiltonian H_I;
  - Transform system adiabatically from H_I to H_P (slowly change *s* from 0 to 1);
  - Measure state of the system to obtain a low-energy solution to P.
- Adiabatic model computationally equivalent to gate model.
- Running time is $O(g_{min}^{-2})$, where g_{min} is the minimum spectral gap of $H(s)$.
  - Inverse gap (g_{min}^{-1}) is exponential for the hardest problems.

Quantum annealing (QA)

- Implementation of the adiabatic quantum computing idea
- QA computers commercially available from D-Wave systems
- Solves optimization problems of the type

$$\text{Minimize} \sum_i a_i x_i + \sum_{i<j} b_{ij} x_i x_j$$

- Running time of order of microseconds
- Not equivalent (weaker) than the gate model
- Why is it called quantum annealing?

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Annealing: simulated vs quantum

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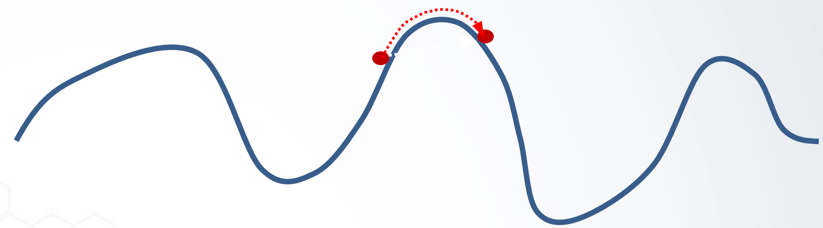
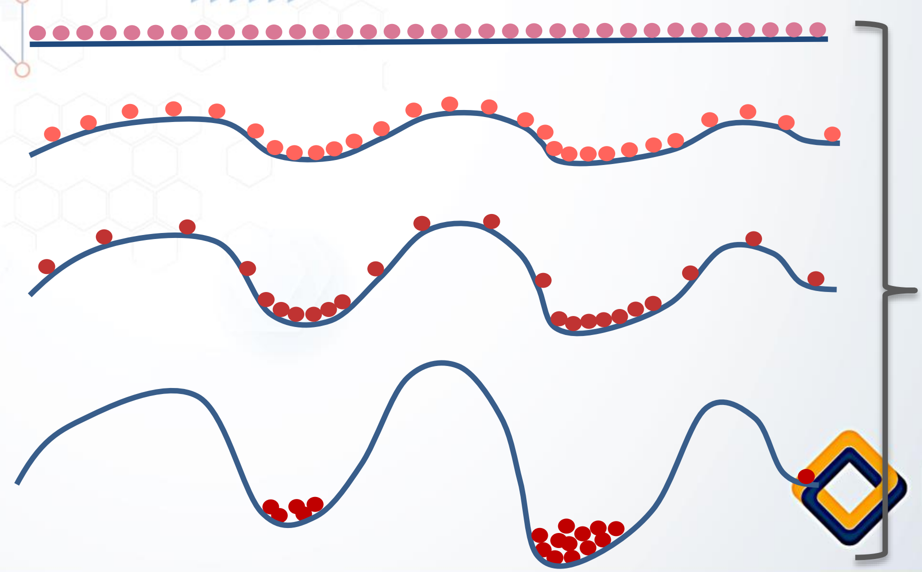
- Simulated annealing: uses thermal effects



- Quantum annealing: quantum effects (Adiabatic Theorem):

Initial: equal superposition



Final: low energy state for target

How to imple-ment that?

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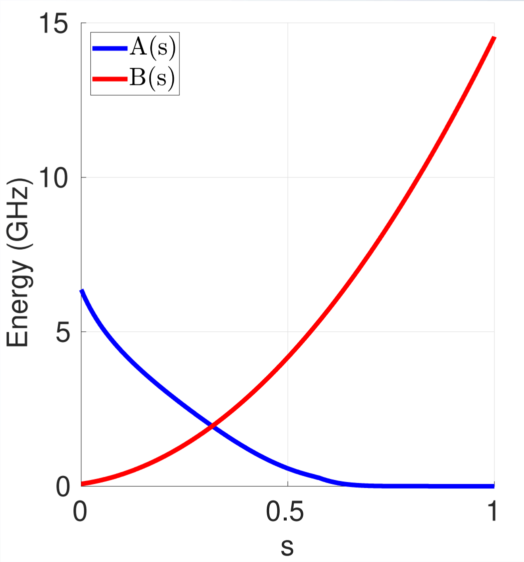
The time-dependent Hamiltonian used for quantum annealing

- Mathematical system (optimization problem):

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

- Physical system: Define the initial and problem *Hamiltonians* :

$$\mathcal{H}_{\mathcal{I}} = \sum_i \sigma_i^x, \quad \mathcal{H}_P = \sum_i a_i \sigma_i^z + \sum_{i<j} b_{ij} \sigma_i^z \sigma_j^z$$



- Combine into a final time-dependent Hamiltonian:

$$\mathcal{H}(t) = A(t)\,\mathcal{H}_I + B(t)\,\mathcal{H}_P,$$

$$A(0)=1, A(1)=0;\ B(0)=0, B(1)=1$$

- How can we use this this framework for solving a specific problem?

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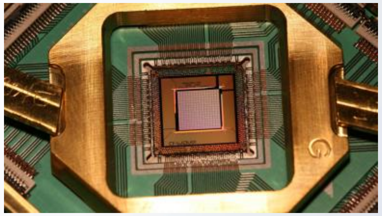
D-Wave computers

- Implements the quantum annealing model
- D-Wave 2000Q at Los Alamos has over 2000 qubits
  - The newest model D-Wave Advantage has over 5000 qubits
- Qubits are implemented as superconducting devices
  - Cooled to about 0.01^0 C above absolute zero
  - Connected by a network *Chimera graph*
  - Annealing time 1–2000 μs
- How to solve a problem on D-Wave?

credit: D-Wave Systems



D-Wave chip

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Combinatorial optimization on D-Wave (from user's perspective)

1. Reformulate the given optimization problem as:

$$\min_{x_1,\ldots,x_n} \left(\sum_{i=1}^{n} a_i x_i + \sum_{1 \le i < j \le n} a_{ij}\, x_i x_j \right)$$

   – Ising formulation: $x_i \in \{-1, 1\}$

   – QUBO formulation: $x_i \in \{0, 1\}$

2. Map problem onto DW hardware

   – Embed connectivity graph defined by a_{ij} coefficients into the quantum hardware graph

   – Encode a_{ij} and a_i coefficients as DW hardware parameters

3. Anneal, read solutions in a loop (500-10,000 times)

Next, we will illustrate the steps with examples.

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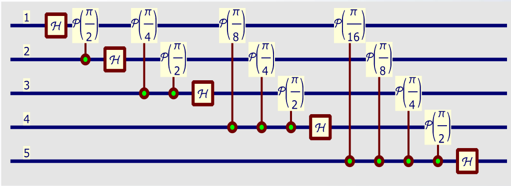
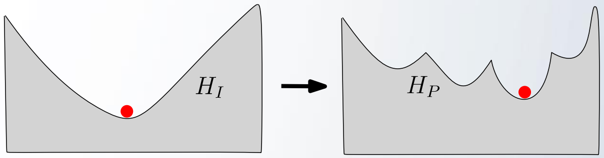
Summary: quantum information and models for quantum computing

- Quantum information
  - Entangled qubits can encode exponential amount of information
  - But that information is very fragile and hard to manipulate
- Gate model quantum computing
  - Analog of a Turing machine, general-purpose
  - Programmed as a sequence of gates



- Adiabatic computing
  - Transition a time-dependent Hamiltonian towards one encoding the solution of the problem in its ground state
  - Theoretically equivalent to the gate-model



- Quantum annealing
  - Practical implementation of the adiabatic computing model
  - Due to very short execution times and hardware noise no optimality can be guaranteed

Examples: solving optimization problems using quantum annealing

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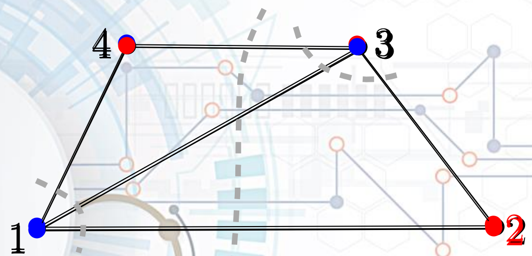
Example 1: Maximum cut problem

- A *cut* in a graph is a partition of its vertices. The size of the cut is the number of edges with endpoints in different sets.
- The Maximum Cut problem asks for a cut of maximum size.



A maximum cut (size 5)

  - NP-hard problem
  - Can also be weighted

- How to solve Max Cut on D-Wave?
  - The first step is to formulate it as a QUBO.

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Step 1. Formulating Max Cut as a QUBO problem

- Define a variable x_i per each vertex i
  - if $x_i = 0$ then i belongs to blue set
  - if $x_i = 1$ then i belongs to red set
- Observe that (i, j) is a cut edge iff $|x_i - x_j| = 1$.
- The size of the cut is then

$$\sum_{(i,j)\in E} (x_i - x_j)^2$$

- QUBO formulation

$$\text{Minimize:} \quad -\sum_{(i,j)\in E} (x_i - x_j)^2 = -\sum_{i\in V} \mathrm{d}(i) x_i + \sum_{(i,j)\in E} x_i x_j$$

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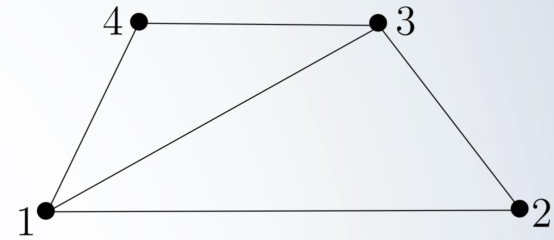
Step 2: Mapping the QUBO to D-Wave processor

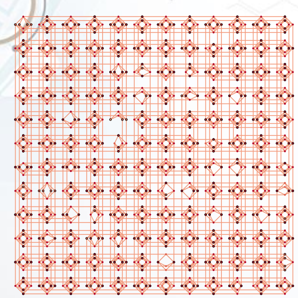
- The QUBO for the example graph



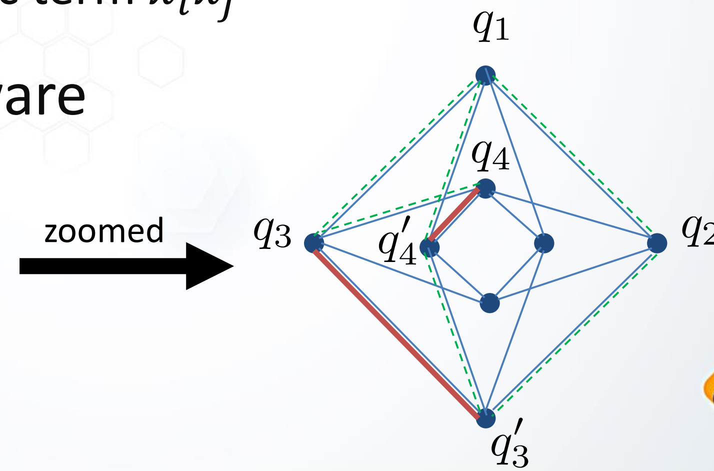
$$Q = -\sum_{i \in V} \mathrm{d}(i) x_i + \sum_{(i,j) \in E} x_i x_j$$

$$= -3x_1 - 2x_2 - 3x_3 - 2x_4 + x_1x_2 + x_1x_3 + x_1x_4 + x_2x_3 + x_3x_4$$

- Construct the graph G defined by Q
  - An edge for each quadratic term $x_i x_j$
- Embed G onto the hardware graph



Chimera graph



Step 3: Running on D-Wave

- Send the QUBO coefficients and parameters to D-Wave
  – Linear (h): [-3,-2,-3,-2]
  – Quadratic (J): {(1,2):1, (1,3):1, (1,4):1, (2,3):1, (3,4):1}
- Parameters for the D-Wave call:
  - h – linear coefficients
  - J – quadratic coefficients
  - annealing_time – between 1 and 2000 μs
  - num_reads – between 500 and 10,000
  - embedding parameters
  - dozens of advanced parameters that are infrequently used

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Step 4. Getting results back and postprocessing

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- If we do 1000 *num_reads*, we get 1000 results called *samples*
- Each sample is converted to a solution to the original problem:
  - Each variable is assigned the value of the corresponding qubit (or chain) measurement
  - If a chain contains both 0 and 1 values, we should decide which one to choose
  - If $x_i = 0$ then we assign i to the blue set and else, we assing i to the red set
  - Compute the size of the cut
- Choose the sample that gives the largest cut.

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Example 2: Maximum clique problem

- A *clique* is a graph with an edge between each pair of vertices.
- The Max Clique problem asks for a subgraph of a given graph that is a clique of maximum size.

  - NP-hard problem with multiple applications

- How to solve Max Clique on D-Wave?
  - The first step is to formulate it as a QUBO.

Solving Max Clique—QUBO formulation

Binary variables: $$x_i = \begin{cases} 1, & \text{if } i \text{ is in the clique;} \\ 0, & \text{otherwise.} \end{cases}$$

<u>Objective</u>: maximize set <u>size</u>:

$$\text{maximize} : \sum_{i \in V} x_i$$

<u>Constraint</u>: vertex set defines a <u>clique</u>:

If $x_i x_j = 1$ then $(i,j) \in E$, or

if $(i,j) \notin E$ then $x_i x_j = 0$.

$$\text{subject to:} \sum_{(i,j) \in \bar{E}} x_i x_j = 0, \quad x_i \in \{0,1\}$$

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QUBO formulation – unconstrained

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1(a) *Constrained* formulation

$$\text{maximize:} \quad \sum_{i\in V} x_i$$

$$\text{subject to:} \quad \sum_{(i,j)\in \bar{E}} x_i x_j = 0, \quad x_i \in \{0,1\}$$

1(b) *Unconstrained* formulation (final)

$$\text{minimize} : -\sum_{i\in V} x_i + M \sum_{(i,j)\in \bar{E}} x_i x_j, \quad x_i \in \{0,1\}$$

2. Mapping the QUBO to the hardware (next)

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Step 2: Mapping the QUBO to D-Wave processor

- The QUBO function

$$Q = -\sum_{i \in V} x_i + M \sum_{(i,j) \in \bar{E}} x_i x_j, \quad x_i \in \{0,1\}$$

- Construct the graph G(Q) defined by *Q*
  - G(Q) is a near-complete graph even if the input graph is sparse
- Embed *G* onto the hardware graph (Chimera)
  - The size of problems that can be solved on DW 2000Q limited to ~65

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How well does it work?

- Depends on the problem and the size of the graph
  - Max Clique is usually easier to solve than Max Cut
  - For larger graphs (near the limits of the hardware) optimal solution are often harder to find
  - Accuracy depends also on the density (# of edges)
  - For smaller size (say 40 vertices or less) DW usually finds an optimal solution
- Depends on the current state of the quantum hardware (noise, etc.)
- Using advanced features of D-Wave and hybrid classical-quantum algorithms may help

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Conclusions

- Quantum computing holds a long-term promise, but current technology (Noisy Intermediate-Scale Quantum (NISQ)) needs a lot of improvement.
- *Quantum annealing* is the model that currently offers largest number of qubits and is easiest to program
  - Commercially available from D-Wave Systems
  - For solving optimization problems
  - Upto 5000 qubits (7000 qubits in the next model)
  - Still cannot beat conventional computers/algorithms, so using advanced algorithmic/programming methods and features can help close the gap (next lecture)

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