## 18-819F: Introduction to Quantum Computing 47-779/47-785: Quantum Integer Programming \& Quantum Machine Learning

Quantum Annealing, Quantum-Inspired Heuristics, Benchmarking, and Parameter setting
Lecture 14
2021.10.21

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## Quantum Approximate Optimization Algorithm: RECAP



Now if you measure, the probability of a bitstring depends both on $\gamma$ and $\beta$ in a non-linear way.
It is exponentially difficult to predict or simulate the probability
$\left|\mathrm{B}_{2 s}\left(\beta_{1}, \gamma_{1}, \beta_{2}, \gamma_{2}, \ldots, \beta_{p}, \gamma_{p}\right)\right|^{2}$ to find the optimal unknown solution $s^{*}$

$$
\begin{aligned}
& |\psi\rangle_{\mathrm{QAOA}(p)} \\
& =\left(2^{N / 2}\right)^{-1} \sum_{s} \mathrm{~B}_{2 s}\left(\beta_{1}, \gamma_{1}, \beta_{2}, \gamma_{2}, \ldots, \beta_{p}, \gamma_{p}\right) e^{i \Gamma_{1 s}\left(\beta_{1}, \gamma_{1}, \beta_{2}, \gamma_{2}, \ldots, \beta_{p}, \gamma_{p}\right)}|S\rangle
\end{aligned}
$$



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## Quantum Approximate Optimization Algorithm: AWS Braket Excercise

Training of $p=3$ circuit using either quantum simulator or actual quantum hardware

Circuit depth hyperparameter: 3
Problem size: 10
Starting the training.
=========================================================================12 OPTIMIZATION for circuit depth $\mathrm{p}=3$
Param "verbose" set to False. Will not print intermediate steps.

Optimization terminated successfully.
Current function value: -0.937169
Iterations: 2
Function evaluations: 243
Final average energy (cost): -0.937169150437591
Final angles: [4.88261413 2.60870766 2.26309012 1.6607821 1.28592103 2.39641137] Training complete.
Code execution time [sec]: 4.882274389266968
Optimal energy: -6.486032631497276
Optimal classical bitstring: $\left[\begin{array}{llllllllll}-1 & 1 & -1 & -1 & 1 & -1 & 1 & 1 & -1 & -1\end{array}\right]$

Minimal energy found with QAOA: -6.486032631497276


Optimization on graph with $\mathrm{n}=10$ vertices, $\mathrm{m}=20$ edges, optimized with Powell and 10 shots per call; seed=42.



## Stochastic Optimization, Parameters and Statistics of Ising Solvers



1. Set up the quantum algorithm on the QPU with some initial parameters
2. Run it a number of times and process the performance collecting the statistics of distribution
3. If performance is not acceptable, use the distribution to choose new parameters (might involve processing)
$\rightarrow$ Repeat 1-3 until satisfaction
4. Process final result and measure resource used (time, energy)
$\rightarrow$ Repeat 1-4 for many benchmarking instances and collect distribution of performance.
5. Compare against best classical method on available hardware (time, energy)

Congrats, you achieved
quantum
supremacy

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## Quantum and Quantum-Inspired Ising Solvers Examples

1. Quantum Annealing: D-Wave Systems
2. Coherent Ising Machines and Bifurcation Machines

## The Quantum Adiabatic Algorithm for Ising Machines

(1) Map objective function into energy of a quantum Ising system

$$
H_{p}=\sum_{i j} J_{i j} Z_{i} \otimes Z_{j}+\sum_{i} h_{i} Z_{i}
$$

(2) Start from easy problem to solve with known solution

$$
\begin{aligned}
& \boldsymbol{H}_{\boldsymbol{D}}=\Gamma \sum_{i} \boldsymbol{X}_{\boldsymbol{i}} \quad(\text { transverse field }) \\
& |\Psi\rangle_{\text {Nqubits }}=\frac{1}{\sqrt{2^{N}}} \sum_{n=1}^{2^{N}}|\operatorname{solution}(n)\rangle
\end{aligned}
$$

(3) Do any Schrödinger evolution (no measurement! No noise!) that changes the energy states «sufficiently slow».

How slow? It depends on the problem, on $H_{D}$ and on the Annealing Schedule
No way to predict efficiently. Try!

$$
\begin{gathered}
H\left|s_{1} s_{2} \ldots s_{N}\right\rangle=E N\left|s_{1} s_{2} \ldots s_{N}\right\rangle \\
\exp (\boldsymbol{i} \boldsymbol{H})\left|\boldsymbol{s}_{\mathbf{1}} \boldsymbol{s}_{\mathbf{2}} \ldots \boldsymbol{s}_{\boldsymbol{N}}\right\rangle=\boldsymbol{e}^{\boldsymbol{i} \boldsymbol{E}_{\boldsymbol{N}}}\left|\boldsymbol{s}_{\mathbf{1}} \boldsymbol{s}_{\mathbf{2}} \ldots \boldsymbol{S}_{\boldsymbol{N}}\right\rangle \\
X=\left(\begin{array}{cc}
0 & 1 \\
1 & 0
\end{array}\right), \quad Y=\left(\begin{array}{cc}
0 & -i \\
i & 0
\end{array}\right), \quad Z=\left(\begin{array}{cc}
1 & 0 \\
0 & -1
\end{array}\right)
\end{gathered}
$$

$$
\begin{aligned}
& R_{x}(\pi / 2)|0\rangle=|1\rangle \\
& R_{x}(\pi / 2)|1\rangle=|0\rangle
\end{aligned}
$$

If this field is always on and constant the minimum energy state is the all-superposed state


$$
H=A(t) H_{D}+B(t) H_{P}
$$



## Quantum annealing à la D-Wave


( $\rightarrow$ ENGINEERING

$J_{i j}$ and $h_{i}$ have maximum value and fluctuating intrinsic control errors:

$$
\begin{aligned}
& J_{i j}+\delta J \\
& h_{i}+\delta h
\end{aligned}
$$



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## Annealing Schedule Parameters



These are all parameters that influence performance.

reverse annealing time $\tau$

$$
\text { pause time } \rho
$$

First
pause time

Only for elegant problems they can be derived ab-initio. In the real world you have some physics guidance for best guess then you use a heuristics to find them

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## Minor Embedding

## Topological Embedding

( $\mathrm{n}_{\mathrm{H}}$ hardware qubits)


Parameter Setting


$$
\sum_{j \in \in(i)} h_{j}^{\prime}=h_{i}
$$

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$$
\varepsilon(i):\left\{1, \ldots, n_{L}\right\} \rightarrow 2^{\left\{1, \ldots, n_{P}\right\}}
$$

Assign "colors" to connected sets of qubits


$$
J_{j, i, k}^{\prime}<\left\langle h_{i}\right|-\sum_{k=1}^{n} v_{i j} \mid
$$

embedding


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## Minor Embedding of a fully connected graph

Systematic Rule for Embedding

$\mathrm{K}_{4}$

0
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Quadratic overhead


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## Unembedding

$$
\begin{aligned}
& \text { Ferromagnetic Coupling } \\
& f\left(S_{1}, S_{2}\right)=-J F s_{1} s_{2} \\
& f\left(X_{1}, X_{2}\right)=-4 J F\left(-X_{1}-X_{2}+X_{1} X_{2}\right)
\end{aligned}
$$



What is the correct $J_{F}$ ?


Not too large, not too small. Trial and error.
(See Venturelli et al.
https://journals.aps.org/prx/abstract/10.1103/PhysRevX.5.031040)

## Check the AWS Exercises

Let's go to the AWS Braket
https://console.aws.amazon.com/braket Quantum
Annealing tutorials from Quiz III
quantum_annealing/Dwave_Anatomy.ipynb
(also found in GitHub) but if you want to execute it open it in AWS.

- Great background information on
- Quantum Annealing
- Embedding
- Ising Model / MAXCUT / QUBO


## Anatomy of quantum annealing with D-Wave on Amazon Braket

.han notebook dives deep into the anatomy of quantum anneaing wint -Wave on Amazon Brake.
First, the concept of quantum annealing as used by D-Wave is introduced to show how it probabilistically finds the (approximate) optimum to some optimization problem. The nex section intoduces the structures of the D -Wave QPUs and the concept of embedding. Amazon Braket provides two D -Wve devices, 20000 anc Adrantage. The original source graph onto the targe graph. This mapping is called embedding.
Finally, an example QuBO problem is solved using both the classical annealers and QPU to demonstrate the sampling process and a breakdown of the QPU access time.

## Background: quantum annealing

Troduction: On a high level. quantum annealing (QA) is a specific approach to quantum computing, as opposed to the common gate-based model. Quantum annealers are specific-purpose machines designed to solve certain problems belonging to the class of Quadratic Unconstrained Optimization (QUBO) problems. The QUBO mode

 sraket offers access to the superconducting quantum annealers provided by $D$-Wave Systems that can be programmed using the ighh-evel, open sourre tool suite calle ocean.
adiabatic quantum computing makes use of an adiabatic procoess where parameleers are changed sufficienty slow for the system to adapt to the new parameter configuration quasi-instantaneously: For example, in a quantum mechanical system, some Hamiltonian starts trom $H_{0}$ and slowly changes to some o other Hamiltonian $H$ with (tor example) a inear ramp (also called schedule):
wheren $t \in[0$, , $]$ on some time scale. Accordingly, the system's final dynamics at $t=1$ is governed by $H_{1}$ while intitally it is determined by $H_{0}$. If the change in the time dependent Hamilitonian $H(t)$ is sutificientys sow, the resulting dynamics are very simple (accorrding to the adiabatic theorem): it the system starts out in an eigenstate of $H$, the system remains in an instantaneous eigenstate throughout the evolution. Speecifically. If the system started in the ground state (the eigenstate with minimal energy), the
system stays in the ground state, it the condition of adiabaticty (that is related to energy diference between the ground state and the first excted state called the gap) satisfed. This means, to solve a (unknown) ground state of a Hamiltonian for a (hard-t-sosolve) problem, one can start trom an easy-t--solve Hamiltonian with a know ground state.
 heoretical adiabaticty conditions and heuristically repeat the annealing procedure many times, thereby collecting a number of samples tom which the configuration with
 Typically the Hamiltorian $H_{0}$ has the form: $H_{0}=\sum_{i} \sigma_{i}$; with well-known ground state (the equal superposition of all bitstings). And $H_{1}$ is described by the canonoical lising


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## Other exercises on DWave

In AWS Braket https://console.aws.amazon.com/braket there are other interesting Quantum Annealing tutorials quantum_annealing/*

Your plot is saved to maxcut_plot.png


Result to MVC problem: [1, 3, 4, 6, 8, 9]
Size of the vertex cover: 6
(also found in GitHub) but if you want to execute it open it in AWS.

- Classical combinatorial problems: MAXCUT, Graph partitioning, Min vertex cover, Traveling Salesman Person
- Other cases: Factoring, Structural Imbalance

Check (and run) them all

## Minor Embedding - Example

https://colab.research.google.com/github/bernalde/QuIPML/blob/master/notebooks/Notebook\ 7\ -\ DWave.ipynb
From our main example
$\begin{array}{lllllllll}-46 . & 0 & 0 . & 48 . & 48 . & 48 . & 0 . & 48 . & 48.48 .\end{array} 48$.
$0 .-44 . \quad 0.48 . \quad 0.48 .48 . \quad 0.48 .48 .48$.
0. 0. $-44 . \quad 0.48 . \quad 0.48 .48 .48 .48 .48$.
48. 48. $0 .-92.48 .96 .48 .48 .96 .96 .96$
48. 0. 48. 48. -92.48 .48 .96 .96 .96 .96
48. 48. 0. 96. 48. -92 . 48. 48. 96. 96. 96.
0. 48. 48. 48. 48. 48. -91 . 48. 96. 96. 96
48. 0. 48. 48. 96. 48. 48. -92 . 96. 96. 96.
48. 48. 48. 96. 96. 96. 96. 96. -139.144 .144.
48. 48. 48. 96. 96. 96. 96. 96. 144. -138.144.
48. 48. 48. 96. 96. 96. 96. 96. 144. 144. -139 .]

And embed it into a Chimera graph (subgraph of the Chip) Notice that we need to "duplicate" certain variables into several qubits
This step is non-trivial:


Best embedding in 1000 heuristic runs


Full graph embedding

Either use heuristic methods or solve highly constrained problem

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## Coherent Ising Machines


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## NEWS: 100,000 Spins




Fig. 3. MAX CUT score as a function of computation time obtained with the
CIM (orange line) and SA (blue line). The data points exhibit the scores evaluated at the intermediate steps in the CIM and SA computation. The dotted line denotes the score obtained with SG $(10,759,955)$.

ig. 6. Histograms of MAX CUT score with CIM and SA. The vertical dashed line shows the SG score ( $10,759,955$ ).

SCIENCE ADVANCES | RESEARCH ARTICLE
computer science
100,000-spin coherent Ising machine
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## Coherent Ising Machines: Stochastic Differential Equations

Describing the system with zero quantum noise, and neglecting the out-of-phase component of the signal

$$
\dot{x}_{i}=(p-1) x_{i}-x_{i}^{3}+\epsilon \sum_{j} J_{i j} x_{j}
$$

$$
\begin{gathered}
\left(\dot{x}_{i}=\partial V / \partial x_{j}\right) \\
V:=\sum_{i}\left(\frac{(p-1) x_{i}^{2}}{2}+\frac{x_{i}^{4}}{4}\right)-\epsilon \sum_{i j} J_{i j} x_{i} x_{j}
\end{gathered}
$$

$s_{i}=\operatorname{sign}\left(x_{i}\right)$ is
the bit variable

Chaotic-Amplitude-Control (CAC) or Amplitude Heterogeinity Correction or Error-variable Feedback

$$
\begin{aligned}
& \dot{x}_{i}=(p-1) x_{i}-x_{i}^{3}+e_{i} \epsilon \sum_{j} J_{i j} x_{j} \\
& \dot{e_{i}}=-\beta\left(x_{i}^{2}-a\right) e_{i}
\end{aligned}
$$

## Various architectures



FIG. 1: (a) Schematic diagram of the measurement-feedback coupling CIMs with and without the self-diagnosis and dynamic feedback control (closed-loop and open-loop CIMs) indicated using dashed blue and orange lines, respectively. (b) and (c) Dynamical behaviour of the closed-loop and open-loop CIMs, respectively. (b1) and (c1) Inferred Ising energy (the dashed horizontal lines are the lowest three Ising eigen-energies). (b2) and (c2) Mean-field amplitude $\mu_{i}(t)$. (b3) and (c3) Feedback-field amplitude $e_{i}(t)$. (b4) Target squared amplitude $a(t)$. (c4) Pump rate $p(t)$.




## https://arxiv.org/abs/2105.03528

## Coherent Ising Machines: Stochastic Differential Equations



In our simulation, the $x_{i}$ variables are restricted to the range $\left[-\frac{3}{2} \sqrt{\alpha}, \frac{3}{2} \sqrt{\alpha}\right]$ at each time step. The parameters $p$ and $\alpha$ are modulated linearly from their starting to ending values during the $T_{r}$ time steps and are kept at the final value for an additional $T_{p}$ time steps. The initial value $x_{i}$ is set to a random value chosen from a zero-mean Gaussian distribution with a standard deviation of $10^{-4}$ and $e_{i}=1$. Furthermore, 3200 trajectories are computed per instance to evaluate TTS. The actual parameters used for simulation are listed below:

| N step | 3200 |
| :---: | :---: |
| $\Delta T$ | 0.125 |
| $T_{r}$ | 2880 |
| $T_{p}$ | 320 |
| $p$ | $-1.0 \rightarrow 1.0$ |
| $\alpha$ | $1.0 \rightarrow 2.5$ |
| $\beta$ | 0.8 |

Chaotic-Amplitude-Control (CAC) or Amplitude Heterogeinity Correction or Error-variable Feedback

$$
\begin{aligned}
& \dot{x}_{i}=(p-1) x_{i}-x_{i}^{3}+e_{i} \in \sum_{j} J_{i j} x_{j} \\
& \dot{e}_{i}=-\beta\left(x_{i}^{2}-a\right) e_{i}
\end{aligned}
$$

## See for instance:

https://arxiv.org/pdf/2108.07369.pdf

## Oscillation Based Machines, Bifurcation Machines, MemComputers etc.

The Kuramoto Model describes synchronization of oscillators The Toshiba Simulated Bifurcation Machine, Memcomputing




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## Time-to-Solution and variants

- Fix parameters, run many times $\left(\right.$ num $\left._{\text {trials }}\right)$ - estimate $\operatorname{cost} \operatorname{PDF} f\left(x_{i}\right)$
- Define a success test: OK iff cost < target
- Estimation of success probability $P_{\text {success }}=n u m_{\text {OK }} /$ num $_{\text {trials }}=\int \quad d x f(x)=\operatorname{CDF}\left(x_{O K}\right)$
- Probability of succeeding at least once in R attempts: $\mathscr{P}(R) \stackrel{x<x_{0} K}{=} 1-(1-P s u c c e s s)^{R}$
- Invert to find R required to achieve success with at least probability $\mathscr{P}$

$$
\langle\text { TTS }\rangle=\log (1-\mathscr{P}) / \log (1-\text { Psuccess })
$$

Academic Benchmarking Standard: median〈TTS〉(N)



FIG. 2. Pitfalls when detecting speedup. Shown is the
speedup of SOA over SA, defined as the ratio of median time speedup of SQA over SA, defined as the ratio of median time
to find asolution with $9 \%$ probability between SA and SQA
Two cases are presented $a$ both SA and SQA to find a solution with $99 \%$ probability bet ween SA and
Two cases are presented. a) both SA and SQA run optimally
(i.i., the ratio ot the erue scaing curves show in Figure 1).
and there is no asymptotic speedup (solid line). b) SQA (i.e., the ratio of the true scaing curves shown in Figure 1),
and there no asmptoticspedup solid line.) b) SQA is sun
suboptimally at small sizes by choosing a fixed large annealing suboptimally yt small sizes by choosing a fixed large annealing
time $t_{a}=10000$ MCS (dashed ilie). The apparent speedup is, however, due eto suboptimal performance on small sizes
and not indicative of the true asymptotic behavior given by and not indicative of the true asymptotic behavior given by
the solid line, which displays a slowdown of SQA compared
to SA.

## Example 1: CIM vs D-Wave (2020)


https://www.science.org/doi/ 10.1126/sciadv.aau0823


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## Example 2: Sim-CIM vs Adiabatic QAOA

(a) TTS Scalings for 21-Weight Graphs

(b) TTS Scalings as Functions of $\sqrt{n}$ for the SK Model


FIG. 14: Comparison of the time-to-solution (TTS) scalings for the MFB-CIM, DAQC, and DH-QMF in solving MAxCut. (a) Wall-clock time of a closed-loop CIM with a low-finesse cavity ( $\gamma_{\mathrm{s}} \Delta T_{\mathrm{c}}=0.1$ ), DAQC with an optimum number of layers ( $p=20$ ), and DH-QMF with an a priori known number of optimum iterations versus problem size $n$. (b) TTS of the closed-loop CIM on the fully connected SK model for problem sizes from $n=100$ to $n=800$, in steps of 100 . For each problem size, the minimum TTS with respect to the optimization over $t_{\text {max }}$ is plotted. In comparison, the SK model TTSs are shown for 20-layer DAQC and DH-QMF for problem sizes ranging from $n=10$ to $n=20$. The straight, lighter-blue line (a linear regression) for the CIM demonstrates a scaling according to $A B^{\sqrt{n}}$. The lighter-orange and lighter-green best-fit curves for DAQC and DH-QMF are extrapolated to larger problem instances, illustrating a scaling that is exponential in $n$ rather than in $\sqrt{n}$. In both figures, the shaded regions show the IQRs.
https://arxiv.org/abs/2105.03528

## Example 3: D-Wave vs Digital Annealer and Parallel Tempering


https://arxiv.org/abs/2103.08464

FIG. 2. Median optTTS for different solvers for the quadratic 3R3X instances at different problem sizes $n$. The error bars correspond to $2 \sigma$ confidence intervals calculated using a Bayesian-bootstrap. Each solver is represented with a different marker correspond to $2 \sigma$ confidence intervals calculated using a Bayesian-bootstrap. Each solver is represented with a different marke
and color, as denoted by the legend. DAU is Fujitsu's Digital Annealer Unit, run in parallel mode on 25 April 2020. SBM is Toshiba's Simulated Bifurcation Machine, accessed via Amazon Web Services on 20 August 2020. PT is our implementation of parallel tempering. MEM is the Virtual MemComputing Machine. SATonGPU is the data from Fig. 5 of Bernaschi et al. [ $[37]$ after converting their native three-body 3R3X results in $n / 2$ variables to $n$ two-body variables by simplying doubling their reported $n$ values. Note that the SATonGPU results are plotted on a separate, shifted horizontal axis (top, blue), as this solver reached significantly larger problem sizes than the other solvers; its optTTS is smaller by at least two orders of magnitude than
the rest. DWA is the D-Wave Advantage1.1 device accessed via LEAP on 31 October 2020. DWAsub are suboptimal points in the rest. DWA is the D-Wave Advantagel.1 device accessed via LEAP on 31 October 2020 . DWAsub are suboptimal points in
which the optimal runtime is below $1 \mu s$, the lowest runtime possible on the Advantage1.1 device. The lines correspond to the exponential fits [Eq. (3)] of the data, with the coefficients given in Table II. The DWAsub points were not used in computing the DWA scaling exponent reported in Table II.

## Quantum Volume and variants

How large and how long are the programs that a quantum processor can run reliably today?
https://quantum-journal.org/papers/q-2020-11-15-362/



Fidelity of two pure quantum states is a distance metric that could be defined as the overlap/transition probability:

$$
F(\psi, \phi)=|\langle\psi \mid \phi\rangle|^{2}
$$

Can be generalized for noisy quantum states.

## Quantum Volume and variants



## Approximation Ratio as a function of time

## Approximation Ratio

The probability that $R$ variables are all less than $x$ is $F(x)^{R}$
The PDF for the maximum of $R$ iid runs is $=d F / d E=R F_{E}(x)^{R-1} P_{E}(x) E(x)$
For a discrete distribution:

$$
\mathbb{E}\left(Y_{N}\right)=\sum_{k=1}^{L}\left[\left(\sum_{r=k}^{L} p\left(x_{r}\right)\right)^{N}-\left(\sum_{r=k+1}^{L} p\left(x_{r}\right)\right)^{N}\right]_{x_{k}} \text { https:///arxiv.org/pdf//2001.04014.pdf }
$$

Can be obtained by bootstrapping!
Generate $N \gg 1$ runs. Select randomly $R \ll N$. Compute the max of $R$. Repeat and average.

## How to evaluate the parameter setting

In the real world what you care about is «speedup at application scale» for your problem of interest.

R runs at fixed parameters

See exercise on example of Simulated annealing.

## Resources to study

Comparison D-Wave, CIM
Comparison CIM, QA-QAOA
Comparison FujitsuDA, PT, D-Wave
(see slides online for links)

MIMO wireless with D-Wave and with CIM dynamics

## Let's go to Colab

https://colab.research.google.com/github/bernalde/QuIPML/blob/ma ster/notebooks/Notebook\%204\%20-\%20Benchmarking.ipynb
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