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

Ising Model and QUBO problems

Lecture 08

09.28.2022

Quiz 2

What is the optimal objective function value of the following problem?

$$\min_{\mathbf{x}} 2x_0 + 4x_1 + 4x_2 + 4x_3 + 4x_4 + 4x_5 + 5x_6 + 4x_7 + 5x_8 + 6x_9 + 5x_{10}$$

$$s.t. \begin{bmatrix} 1 & 0 & 0 & 1 & 1 & 1 & 0 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 & 1 & 0 & 1 & 1 & 1 \\ 0 & 0 & 1 & 0 & 1 & 0 & 1 & 1 & 1 & 1 & 1 \end{bmatrix} \mathbf{x} = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}$$

$$\mathbf{x} \in \{0,1\}^{11}$$

$$\min \sum_i c_i x_i$$
$$A\mathbf{x} = b$$
$$\mathbf{x} \in \{0,1\}^n$$

What is the optimal objective function of $\min \sum_i \exp(c_i x_i^2)$?

$$A\mathbf{x} = b$$
$$\mathbf{x} \in \{0,1\}^n$$

Which variable(s) is(are) 1 in the optimal solution of $\min \sum_i \log(c_i + x_i)$?

$$A\mathbf{x} = b$$
$$\mathbf{x} \in \{0,1\}^n$$

Quiz 2

- Follow Lecture X in order to create an IBM Qiskit, DWave Leap, and Amazon Web Services account.
- Update a PDF with a proof that you have created each account.

Agenda

- Ising Model: Background, Physics, Definitions, Solutions
- Ising Model and Combinatorial Optimization: MaxCut, QUBO
- QUBO Mappings: equality constraints, inequality constraints, integers to bits, quadratization
- Simulated Annealing

Ising Model

Curiosity

1895, Pierre Curie *(Nobel Prize 1903)* finds that heating a magnet can cause it to lose its magnetic property, i.e., cause a **"phase transition"**.

- But **Why?**

Model

1920 - Lenz introduced a model to explain this phase transition.

1925 - Lenz's student, Ising, solved a special 1-D case of the model

1940 - Onsager *(Nobel Prize 1968)* solves the 2-D case.

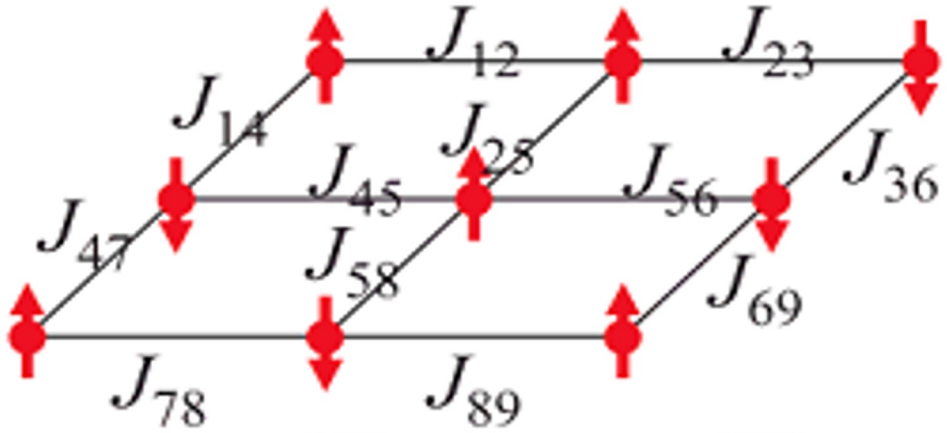
2000 - Istrail shows, via a Max-Cut formulation, that the much sought after 3-D case is NP-Complete

General lesson

1971 - Wilson *(Nobel Prize 1982)*, **Universality**: Systems with same number of dimensions and symmetries go through identical phase transitions.

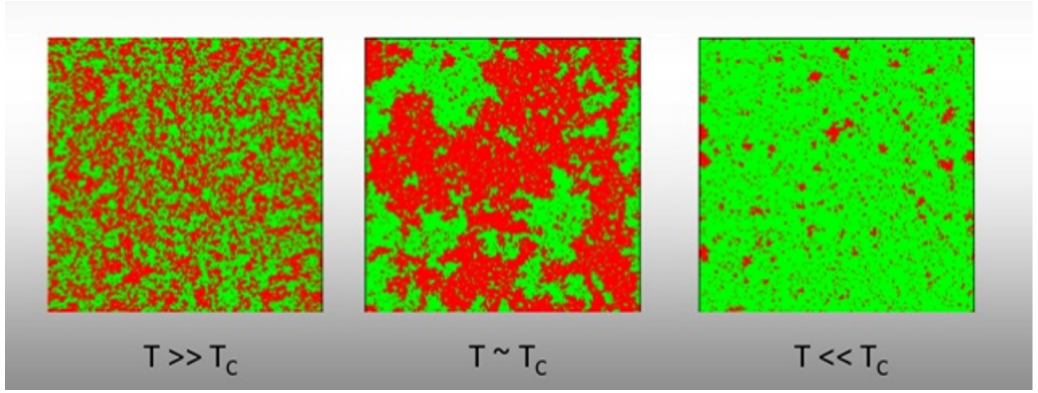
Ising is the simplest model in theory space that captures properties of several interacting systems like magnets, water etc.

Ising Model Magnetic Phenomenology



$$H = -\sum_{\langle i,j \rangle} J_{ij}\sigma_i\sigma_j - \sum_j h_j\sigma_j$$

Spin are subject to thermal fluctuations and can be up or down



Depending on the temperature the fluctuations have macroscopic properties of symmetry ("thermodynamic phases") which are encapsulated in the value of an order parameter ("magnetization")

[1] https://en.wikipedia.org/wiki/Ising_model

Ising Model Definitions and Nomenclature

Mathematical definition

$$H(\sigma) = -\sum_{(ij)\in E(G)} J_{ij}\sigma_i\sigma_j - \mu\sum_{i\in V(G)} h_i\sigma_i$$

- H Energy function or Hamiltonian
- $\sigma_i \in \{-1,+1\}^{V(G)}$ Spin Variables for each site in the graph or lattice
- $G=(V,E)$ Graph or Lattice defining the interactions
- μ Magnetic moment
- $J_{ij}\begin{cases} >0, & \text{ferromagnetic interaction} \\ <0, & \text{antiferromagnetic interaction} \\ =0, & \text{no interaction} \end{cases}$
- $h_i\begin{cases} >0, & \text{site wanting to align with external field} \\ <0, & \text{site wanting to anti-align with external field} \\ =0, & \text{no external influence on site} \end{cases}$

(Quadratic)

Couplings/interactions

Zeeman term, external longitudinal term, bias, ...

Important Examples
- Tree
- Triangle-free graphs
- Planar graph (e.g. square lattice)
- Regular Graph (e.g. 3-regular Erdos-Reiny random graph)
- **Fully Connected/Complete Graph (Sherrington-Kirkpatrick Model)**

- Configuration (Boltzmann) probability: $P(\sigma,\beta) = e^{-\beta H(\sigma)}/Z(\beta)$
- Inverse temperature: $\beta = (k_B T)^{-1}$
- Partition function: $Z(\beta) = \sum_\sigma e^{-\beta H(\sigma)}$ (normalization in probability)

Ising Model - Solutions

"Solving the Model"

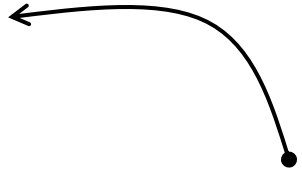
Physicists: identifying the value of thermodynamics expectation values (find the thermal distribution of energies)

Optimization People: find the actual bitstring that minimizes the objective function (find the ground state)

Note: At T=0 only the ground state contributes to the statistics

Known Analytical Solutions

- 1D chain or short range disordered, without external field also quantum.
- 2D not disordered is solvable for thermodynamic phases
- 3D+ case disordered is NP-Hard

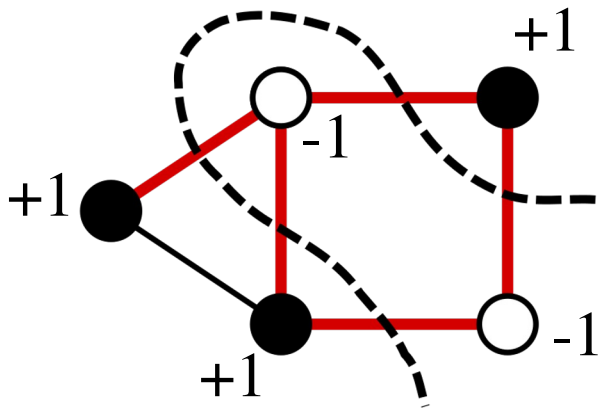


Most of the work is focused on this since we understand everything – but does it generalize?
NO! But it might guide some ideas to be verified empirically.

Ising for Combinatorial Optimization: MaxCut

Starting from Ising Problem without external field

$$
\begin{aligned}
H(\sigma) &= -\sum_{(ij)\in E(G)} J_{ij}\sigma_i\sigma_j \\
&= -\sum_{(ij)\in E(V^+)} J_{ij} - \sum_{(ij)\in E(V^-)} J_{ij} + \sum_{(ij)\in \delta(V^+)} J_{ij} \\
&= -\sum_{(ij)\in E(G)} J_{ij} + 2\sum_{(ij)\in \delta(V^+)} J_{ij}
\end{aligned}
$$



where the set V^+ (V^-) are all the vertices with $\sigma = +1\,(\sigma = -1)$ and their boundary (cut) is denoted by $\delta(V^+)$

Now consider that the graph has weighted edges W_{ij}

Then the size of the cut is $|\delta(V^+)| = \frac{1}{2}\sum_{(i,j)\in\delta(V^+)} W_{ij}$

Therefore we obtain $H(\sigma) = \sum_{(ij)\in E(G)} W_{ij} - 4|\delta(V^+)|$

When minimizing the Ising model, we are finding the maximum cut of the graph

$$\min_\sigma H(\sigma) = \sum_{(ij)\in E(G)} W_{ij} + 4\max_\sigma |\delta(V^+)|$$

Optimization value of the choice made for the spins

Constant of the problem, easy to compute

[1] https://www.electronics-tutorials.ws/electromagnetism/magnetism.html
[2] http://www.irm.umn.edu/hg2m/hg2m_b/hg2m_b.html

From Ising to Quadratic Binary Unconstrained (QUBO)

Starting from the minimization of the Ising Model

$$\min_{\sigma\in\{-1,+1\}^n} H(\sigma) = \min_{\sigma\in\{-1,+1\}^n} \sum_{(ij)\in E(G)} J_{ij}\sigma_i\sigma_j + \sum_{i\in V(G)} h_i\sigma_i$$

We can directly pose this problem as a Quadratic Unconstrained Binary Optimization (QUBO).

$$\min_{\sigma\in\{-1,+1\}^n} \sum_{(ij)\in E(G)} J_{ij}\sigma_i\sigma_j + \sum_{i\in V(G)} h_i\sigma_i =$$
$$\min_{\mathbf{x}\in\{0,1\}^n} \sum_{(ij)\in E(G)} x_i Q_{ij} x_j + \sum_{i\in V(G)} Q_{ii}x_i + c$$

with $Q_{ij} = 4J_{ij}, Q_{ii} = 2h_i - \sum_{j\in V(G)}(2J_{ij}+2J_{ji}), c = \sum_{i<j} J_{ij} - \sum_{i\in V(G)} h_i$

$$J_{ij} = Q_{ij}/4, h_i = Q_{ii}/2 + \sum_{j\in V(G)}(Q_{ij}/4 + Q_{ji}/4), c_I = c_Q + \sum_{i<j} Q_{ij}/4 - \sum_{i\in V(G)} Q_{ii}/2$$

EXERCISE: put this in ILP form introducing the variable $x_{ij} = x_i x_j$

$$\sigma_i = 2x_i - 1 \qquad x_i = (\sigma_i + 1)/2$$
$$\sigma_i\sigma_j = 4x_ix_j - 2x_i - x_j + 1 \iff x_ix_j = (\sigma_i\sigma_j + \sigma_i + \sigma_j + 1)/4$$

QUBO model

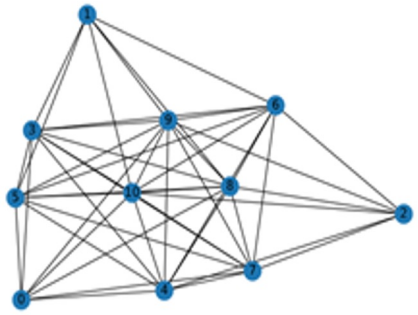
Quadratic Unconstrained Binary Optimization

$$\min_{\mathbf{x}\in\{0,1\}^n} \sum_{(ij)\in E(G)} x_i Q_{ij} x_j + \sum_{i\in V(G)} Q_{ii} x_i + c$$
$$= \min_{\mathbf{x}\in\{0,1\}^n} \mathbf{x}^\top \mathbf{Q}\mathbf{x} + c$$

Quadratic coefficient matrix $\mathbf{Q}$

- Can be either upper triangular or complete $x_i x_j = x_j x_i$
- Elements on diagonal can be linearized $x_i^2 = x_i$ if $x_i \in \{0, 1\}$
- Represents adjacency matrix of a problem

$$\begin{bmatrix}
-46. & 0. & 0. & 48. & 48. & 48. & 0. & 48. & 48. & 48. & 48. \\
0. & -44. & 0. & 48. & 0. & 48. & 48. & 0. & 48. & 48. & 48. \\
0. & 0. & -44. & 0. & 48. & 0. & 48. & 48. & 48. & 48. & 48. \\
48. & 48. & 0. & -92. & 48. & 96. & 48. & 48. & 96. & 96. & 96. \\
48. & 0. & 48. & 48. & -92. & 48. & 48. & 96. & 96. & 96. & 96. \\
48. & 48. & 0. & 96. & 48. & -92. & 48. & 48. & 96. & 96. & 96. \\
0. & 48. & 48. & 48. & 48. & 48. & -91. & 48. & 96. & 96. & 96. \\
48. & 0. & 48. & 48. & 96. & 48. & 48. & -92. & 96. & 96. & 96. \\
48. & 48. & 48. & 96. & 96. & 96. & 96. & 96. & -139. & 144. & 144. \\
48. & 48. & 48. & 96. & 96. & 96. & 96. & 96. & 144. & -138. & 144. \\
48. & 48. & 48. & 96. & 96. & 96. & 96. & 96. & 144. & 144. & -139.
\end{bmatrix}$$



Offset c

- Irrelevant for optimization

In terms of IP it would be a

Non-convex Integer Nonlinear Program

QUBO Mappings Examples: Linear Equality Constraints

Example: Binary Linear Programming

$$\min_{\mathbf{x}\in\{0,1\}^n} \mathbf{c}^\top \mathbf{x}$$

$$s.t.\ \mathbf{Ax} = \mathbf{b}$$

Hard Constraint

$\min(H) \Leftrightarrow H_A = 0$

Objective Function to be optimized

We can write the energy function in two terms $H = H_A + H_B$

- Constraint satisfaction $(H_A = 0)$

$$H_A = \rho \sum_{j=1}^{m} \left(\sum_{i=1}^{n} A_{ij} x_i - b_j \right)^2$$

Penalty Coefficient

- Objective function

$$H_B = \sum_{i=1}^{n} c_i x_i$$

How to determine the penalty? Guarantee that the minimal >0 value for H_A is larger than the gap between the ground state of H_B and the minimum energy that satisfies the constraint (unknown – but can be bound)

Note: another method to use is through Lagrange multipliers (see previous lectures)

[1] Bian, Zhengbing, et al. "Discrete optimization using quantum annealing on sparse Ising models." Frontiers in Physics 2 (2014): 56.

[2] Lucas, Andrew. "Ising formulations of many NP problems." Frontiers in Physics 2 (2014): 5.

QUBO Mappings Examples: Polynomial Unconstrained Binary (PUBO)

Any pseudo-Boolean function defined as

$$f : \{0,1\}^n \mapsto \mathbb{R}$$

Can be written uniquely as a sum of multilinear functions

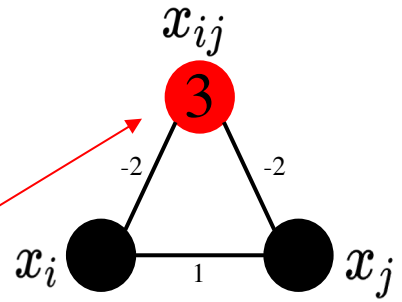
$$f(x) = a_0 + \sum_i a_i x_i + \sum_{ij} a_{ij} x_i x_j + \sum_{ijk} a_{ijk} x_i x_j x_k + \dots$$

We can transform any binary polynomial into a quadratic polynomial by introducing new variables as we

$$x_{ij} = x_i x_j$$

Naive example:

- Using linear inequalities
  $$x_{ij} \geq x_i + x_j - 1, x_{ij} \leq x_i, x_{ij} \leq x_j$$
- Using a polynomial expression as penalty (gadget)
  $$H(\mathbf{x}) = 3x_{ij} + x_i x_j - 2x_{ij} x_i - 2x_{ij} x_j$$



Usually called ancillary variables

x_i	x_j	x_{ij}	$x_i x_j$	$H(\mathbf{x})$
1	1	1	1	0
1	1	0	1	1
1	0	1	0	1
1	0	0	0	0
0	1	1	0	1
0	1	0	0	0
0	0	1	0	3
0	0	0	0	0

[1] Babbush, Ryan, Bryan O'Gorman, and Alán Aspuru-Guzik. "Resource efficient gadgets for compiling adiabatic quantum optimization problems." Annalen der Physik 525.10-11 (2013): 877-888.

[2] Boros, Endre, and Peter L. Hammer. "Pseudo-boolean optimization." Discrete applied mathematics 123.1-3 (2002): 155-225.

Ising Model and Integer Programming Hands-On

https://colab.research.google.com/github/bernalde/QuIPML22/blob/main/notebooks/Notebook%202%20-%20QUBO%20and%20Ising.ipynb

QUBO Mappings Examples: From Integers to Bits

How to transform general Integer Programs into Binary programs?

$$y \in \{0, \cdots, \bar{y}\} \subseteq \mathbb{Z}$$

In general with a width of the integer encoding d

$$y = \sum_{j=1}^{d} k_j x_j = \mathbf{k}^\top \mathbf{x}, k_j \in \mathbb{Z}_+, x_j \in \{0, 1\}$$

- Unary encoding $k_j = 1, d = \bar{y}$
- Binary encoding $k_j = 2^{j-1}, d = \lfloor \log_2(\bar{y}) \rfloor$
- Bounded encoding

We can find an encoding with an upper bound for the coefficients $\mu \ll \bar{y}$

if $\bar{y} < 2^{\lfloor \log(\mu) \rfloor} + 1$ if $\bar{y} > 2^{\lfloor \log(\mu) \rfloor} + 1$

N bits for 1…N
Min precision req

$\log_2$(N) bits for 1…N
max precision req

[1] Karimi, Sahar, and Pooya Ronagh. "Practical integer-to-binary mapping for quantum annealers." Quantum Information Processing 18.4 (2019): 94.

QUBO Mappings Examples: Linear Inequality Constraints

For linear equality constraints

$$s.t.\ \mathbf{Ax} = \mathbf{b} \longrightarrow H_A = \rho \sum_{j=1}^{m} \left(\sum_{i=1}^{n} A_{ij} x_i - b_j \right)^2$$

Inequality constraints:

$$\boldsymbol{Ax} \leq \boldsymbol{b}$$
$$\boldsymbol{Ax} - \boldsymbol{b} \leq \mathbf{0}$$
$$\boldsymbol{Ax} + \boldsymbol{s} - \boldsymbol{b} = \mathbf{0}$$

"slack variable"
Free variable that can take any value from zero to b

⟺

As long as $Ax \leq b$ there is one value of s that satisfies the equality constraint

Typical situation in mappings:
(e.g. knapsack problem)

$$\sum_i x_i \leq M$$
$$\sum_i x_i + \sum_j m_j y_j = M$$
$$H_A = \rho \left(\sum_i x_i + \sum_j m_j y_i - M \right)^2$$

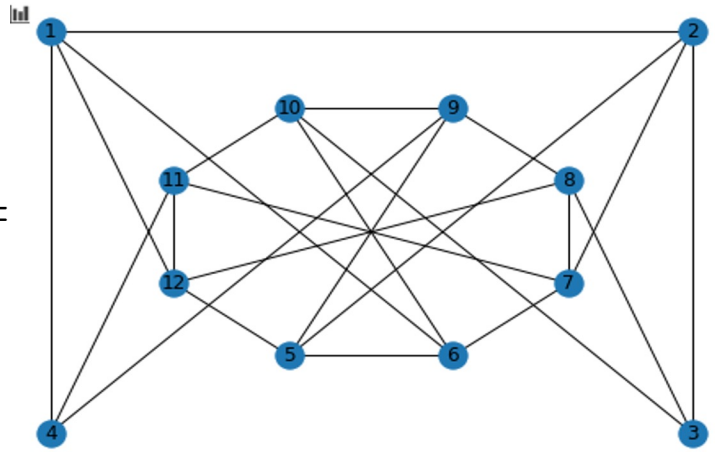
From integers to bits

QUBO Mappings Examples: Graph Coloring

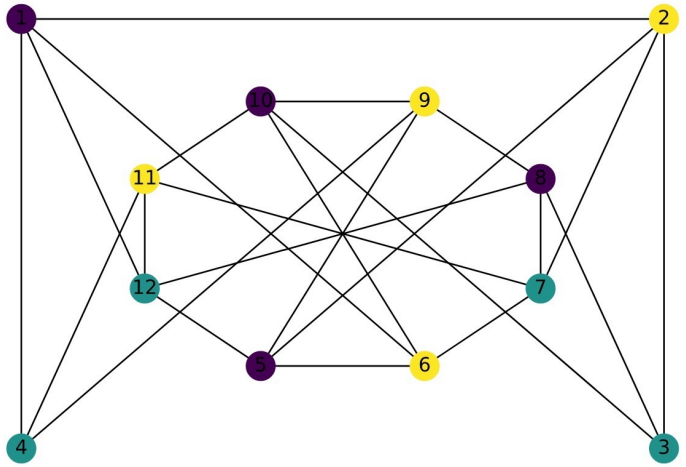
Coloring with colors $K = \{1, \cdots, k\}$

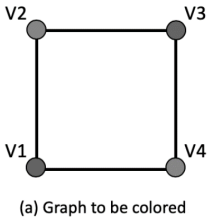
x_{ij} = is node i colored with color j?

$\mathcal{G}(V, E) =$

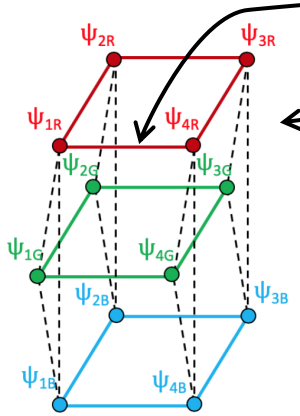


3-coloring





(a) Graph to be colored



$$H_A \quad \min_{\mathbf{x}} \sum_{i \in V} \left(1 - \sum_{j \in K} x_{ij}\right)^2 + \sum_{(uv) \in E} \sum_{j \in K} x_{uj} x_{vj}$$

$$x_{ij} \in \{0, 1\}, \forall j \in K, \forall i \in V$$

QUBO/PUBO Mappings Examples: Literature

REVIEW article
Front. Phys., 12 February 2014 | https://doi.org/10.3389/fphy.2014.00005

Ising formulations of many NP problems

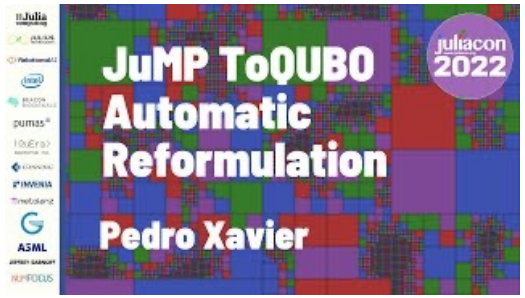
Andrew Lucas*
Lyman Laboratory of Physics, Department of Physics, Harvard University, Cambridge, MA, USA

EXERCISE: study the Traveling Salesman Problem Mapping

☆ 99 Cited by 897 Related articles All 12 versions »

Follow on google scholar citing articles to discover mappings of many industrially relevant combinatorial optimization problems. (The paper of Lucas has some typos and some mappings are inefficient)

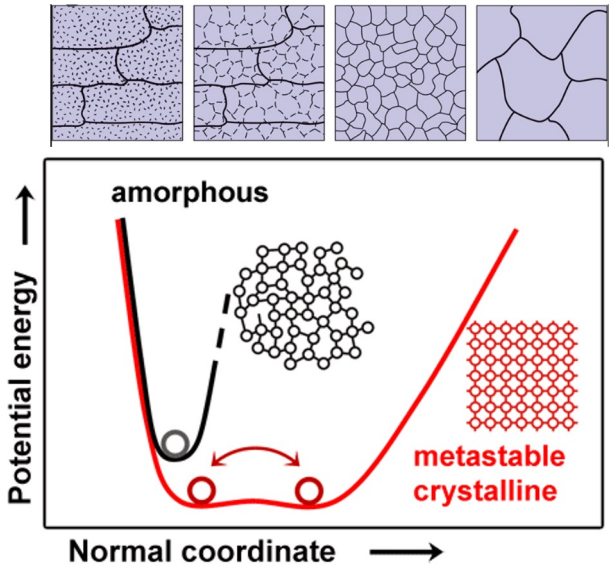
See software that does mappings automatically:
toQUBO.jl
PyQUBO https://arxiv.org/abs/2103.01708
D-Wave Ocean https://docs.ocean.dwavesys.com/en/stable/
IBM https://qiskit.org/documentation/apidoc/qiskit_optimization.html
also commercial quantum startups are releasing software products:
e.g. Quantum Computing Inc. Qatalist; QC-Ware Forge



ToQUBO.jl

psrenergy/
ToQUBO.jl
JuMP ToQUBO Automatic Reformulation
2 Contributors 8 Issues 9 Stars 1 Fork

Simulated Annealing



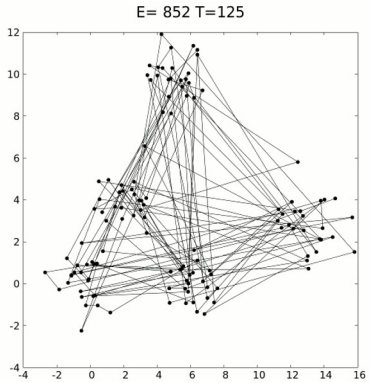
Concept coming from annealing in metallurgy

Slow cooling allows for perfect crystals (minimizing energy)

Start at effective high temperature and gradually decrease the temperature by increments until is slightly above zero

Interesting behavior:

- "Divide-and-conquer": Big features are solved early in the search and small features later while refining
- Ability to escape local-minima
- Guaranteed to reach lowest energy if temperature is lowered slowly enough



[1] Scott Kirkpatrick, C Daniel Gelatt, and Mario P Vecchi. Optimization by simulated annealing.Science,220(4598):671–680, 1983.
[2] https://www.esrf.eu/news/general/phase-change-materials/index_html
[3] Alan Lang Chapter 8 Strain hardening and annealing.

Ising Model – Monte Carlo, Physics Inspired Methods

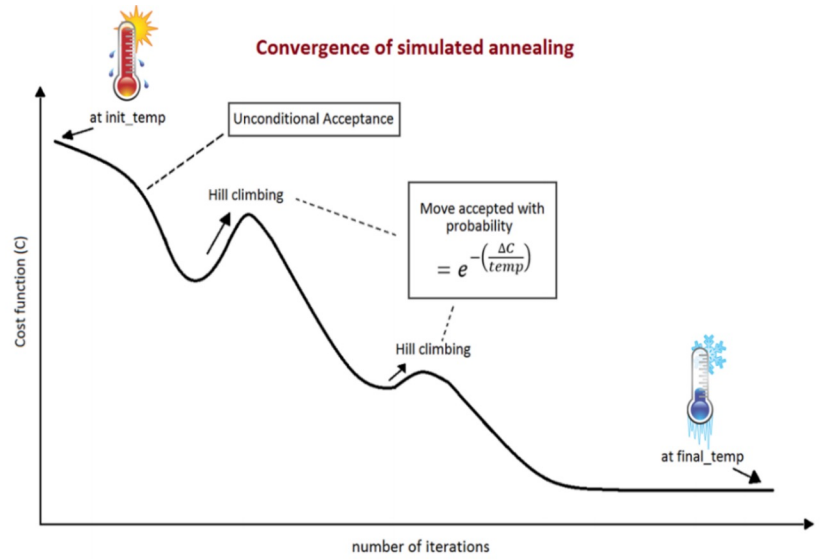
Ising model as Markov-Chain

The immediate probability $P(\boldsymbol{\sigma}^c, \beta) = e^{-\beta H(\boldsymbol{\sigma}^c)} / Z(\beta)$ of transitioning to a future state $\boldsymbol{\sigma}^f$ depends only in the current state $\boldsymbol{\sigma}^c = [\sigma_1^c, \cdots, \sigma_N^c]$

Given single flip dynamics, we can jump from any state to another.

Metropolis-Hastings Monte Carlo Algorithm for Ising Models

1) Start with a known configuration, $\boldsymbol{\sigma}^i = [\sigma_1^i, \cdots, \sigma_N^i]$ corresponding energy $H(\boldsymbol{\sigma}^i)$ and temperature value $T = (k_B\beta)^{-1}$
2) Randomly change the configuration
   - Flip some spins $\sigma^i \rightarrow \sigma^j$
1) Calculate new energy value $H(\boldsymbol{\sigma}^j)$
2) Compare to energy at previous position
   - If , $H(\boldsymbol{\sigma}^j) < H(\boldsymbol{\sigma}^i)$ keep new position
   - If , $H(\boldsymbol{\sigma}^j) > H(\boldsymbol{\sigma}^i)$ keep new position if Boltzmann factor for transition satisfies $\exp\left[-\frac{H(\boldsymbol{\sigma}^j) - H(\boldsymbol{\sigma}^i)}{k_B T}\right] \geq \text{Rand}[0, 1]$
1) Repeat 2) - 4) K times



[1] Scott Kirkpatrick, C Daniel Gelatt, and Mario P Vecchi. Optimization by simulated annealing.Science,220(4598):671–680, 1983.

Ising Model – Mathematical background

$$\mathcal{H}(\bar{\sigma}) = \underbrace{\sum_{i<j} J_{ij}\sigma_i\sigma_j}_{\text{Interaction}} + \underbrace{\sum_{i} h_i\sigma_i}_{\text{Local field}}$$

$$\mathcal{Z} = \sum_{\bar{\sigma}\in\{0,1\}^n} e^{-\beta\mathcal{H}(\bar{\sigma})}$$

$$\mathcal{F} = -\frac{1}{\beta}\ln\mathcal{Z} = \langle\mathcal{H}\rangle - T\mathcal{S}$$

- **Ising model** represents the microscopic interaction of magnetic spins, with $\sigma = \pm 1$
- The most important quantity to compute is the ***Partition Function*** $\mathcal{Z}$
- Thermodynamic quantities can be computed from the ***Free Energy*** $\mathcal{F}$

Mandra, S. Lecture on Ising Models, 2021

Simulated Annealing

$$p(\bar{\sigma}) = \frac{e^{-\beta \mathcal{H}(\bar{\sigma})}}{\mathcal{Z}}$$

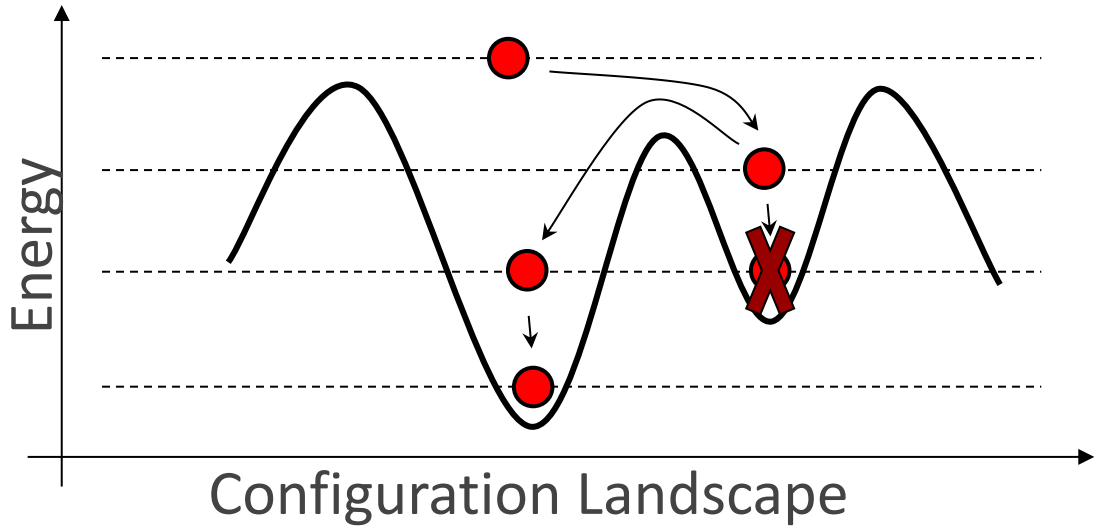
- **How to sample** from the Gibbs distribution?
- Metropolis & Hastings devised a **Markov-Chain Monte Carlo** algorithm to sample from $p(\bar{\sigma})$
- **Simulated annealing** is an adaptation of MH algorithm by slowly lowering the temperature from high (paramagnetic) to zero

Mandra, S. Lecture on Ising Models, 2021

Simulated Annealing

- For a sufficiently **large number of steps**, the spin system will reach "**thermalization**" and therefore, configurations are sampled accordingly to the **Gibbs distribution**.
- Starting from **high temperature** and then **slowly reducing it**, the system will **eventually thermalize** at any given temperature and therefore, **sample the ground state**.

Using the Metropolis-Hasting algorithm to compute the transition probability $p(\sigma'|\sigma)$, **preserving both the detailed balance and ergodicity of the system,** would eventually **drive the system** to a given stationary distribution $p(\sigma)$.



Mandra, S. Lecture on Ising Models, 2021

Simulated Annealing Exercise

https://colab.research.google.com/github/bernalde/QuIPML22/blob/main/notebooks/Notebook%202%20-%20QUBO%20and%20Ising.ipynb

Preview: Advanced Simulated Annealing

As seen before, the displacement δ is key to performance.

In naive Simulated annealing the displacement can be a "single flip" $\delta : \sigma_i \mapsto -\sigma_i$

- For hard optimization problem this might require exponential time to converge.

What if the update happens between "clusters" of spins?

- This needs to be done carefully to guarantee energy conservation and ergodicity
  - In this context that one can reach any state from another given the Markov-chain
- Generate different replicas of the system at different temperatures and after certain Metropolis updates, the temperatures of two replicas r_1, r_2 are exchanged if

$$P(r_1 \leftrightarrow r_2) = \min\{1, \exp[(\beta_1 - \beta_2)(H(\sigma^1) - H(\sigma^2))]\}$$

  - Two temperatures are always exchanged if a replica at higher temperature has a lower energy than a replica with a lower temperature.
  - Otherwise, the exchange of the two temperatures is either accepted or rejected using the random number between 0 and 1

[1] S. Mandra, Z. Zhu, W. Wang, A. Perdomo-Ortiz, H. G. Katzgraber. Strengths and weaknesses of weak-strong cluster problems: A detailed overview of state-of-the-art classical heuristics versus quantum approaches. Physical Review A, 94(2), 022,337, 2016.

Parallel Tempering

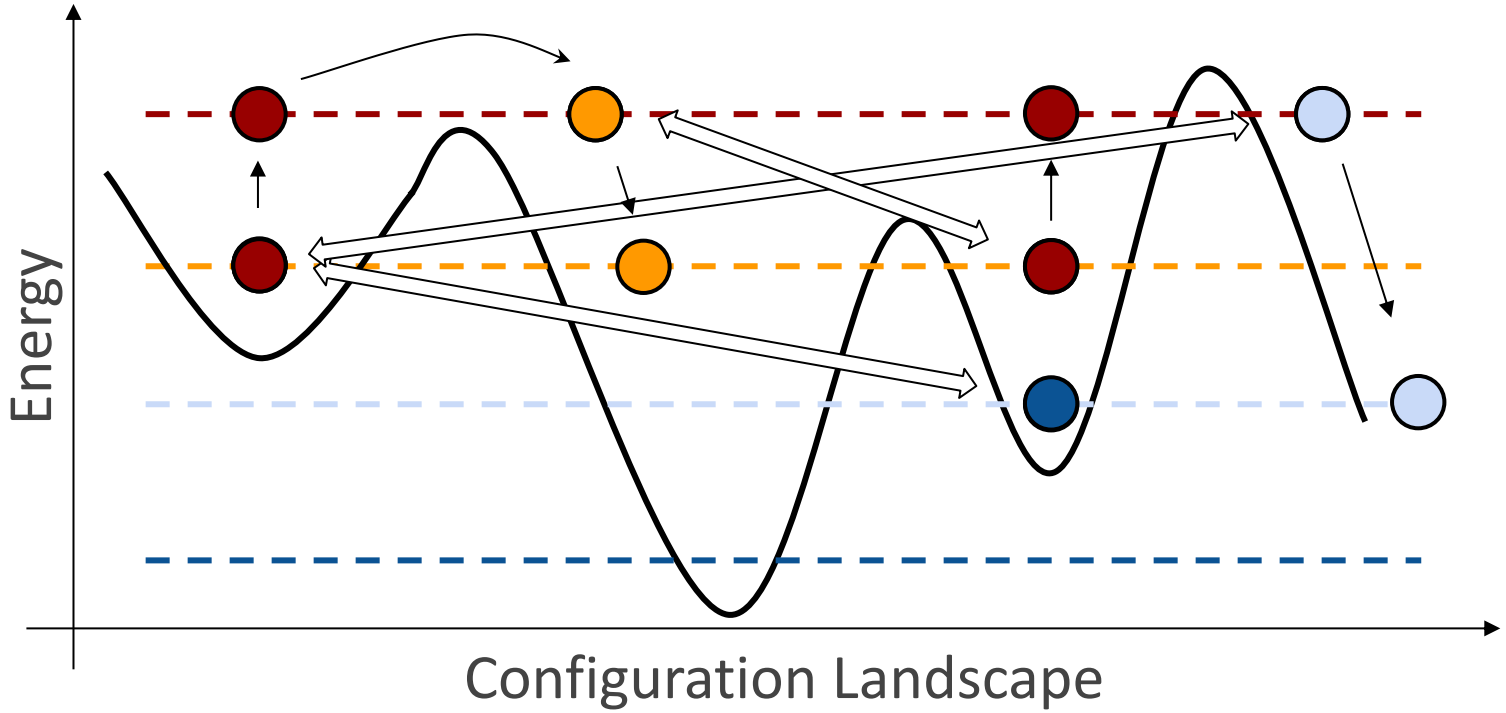
- To avoid being stuck in local minima, replica exchange methods (like parallel tempering) can be used.
- The idea behind parallel tempering is simple: many different replicas at a "fixed" temperature are simulated at the same time.
- After a given number of MH steps, two replicas "exchange temperature" with probability (derivation follows from MH):

$$A_{\text{exchange}} = \min\left\{1, e^{\Delta\beta\Delta\mathcal{H}}\right\}$$

- Replica exchange preserves the detailed balance and ergodicity of the spin system.

Mandra, S. Lecture on Ising Models, 2021

Parallel Tempering



$$A_{\text{exchange}} = \min\left\{1, e^{\Delta\beta\Delta\mathcal{H}}\right\}$$

Mandra, S. Lecture on Ising Models, 2021

[1] S. Mandra, Z. Zhu, W. Wang, A. Perdomo-Ortiz, H. G. Katzgraber. Strengths and weaknesses of weak-strong cluster problems: A detailed overview of state-of-the-art classical heuristics versus quantum approaches. Physical Review A, 94(2), 022,337, 2016.

Preview: How to evaluate heuristics?

This is not a trivial question given that methods may have several parameters to tune, run on different hardware or there is no clear absolute metric.

Important metrics are time and solution quality.

Given an algorithm that runs several times, you would like to know how much should it take for you to get a solution with certain success probability.

Metric: Time to solution of expected runtime

$$TTS(m) = m\tau(m)\frac{\log(1-s)}{\log(1-p(m))}$$

- m number of times run, or sweeps in Simulated Annealing
- s success probability after m sweeps
- $p(m)$ probability of success to achieve (usually high $s = 0.99$)
- $\tau(m)$ time it takes to perform a single sweep

- $m\tau(m)$ Time the algorithm runs

It's going to be useful once benchmarking Quantum methods

[1] Venturelli, Davide, et al. "Quantum optimization of fully connected spin glasses." Physical Review X 5.3 (2015): 031040.