Exploring Quantum Annealing and Tunneling: Harnessing their Potential for Independent Set Sampling

Elie Bermot, Simon Apers

Agenda

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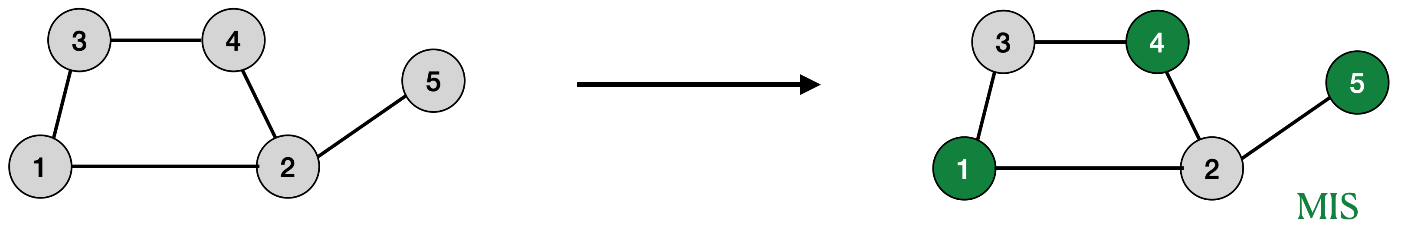
PASQAL

The maximum independent set problem (MIS)



Each node has a label $n_i = \{0; 1\}$

Space of solutions $S = \{0; 1\}^N$ and $|S| = 2^N$

The MIS problem is a NP-complete problem

Associated cost function $C(z_1, \ldots, z_N) = -\sum_{i=1}^{N} n_i + U \sum_{(i,j)\in E} n_i n_j$ with $U \gg 1$

M. R. Garey, D. S. Johnson, Computers and Intractability: A Guide to the Theory of NP-Completeness (WH Freeman & Co., New York, 1979)

Independent sets in bipartite graphs [DFJ02]

Let $G = (L \cup R,\ E), |L| = |R| = n$ be a Δ −regular bipartite graph

Definition: We define $I(\alpha, \beta)$ as the set of independent sets of G with αn vertices in L and βn vertices in R.

Definition: We define

$$\mathcal{E}(\alpha, \beta) := \mathbb{E}_G[|I(\alpha, \beta)|]$$

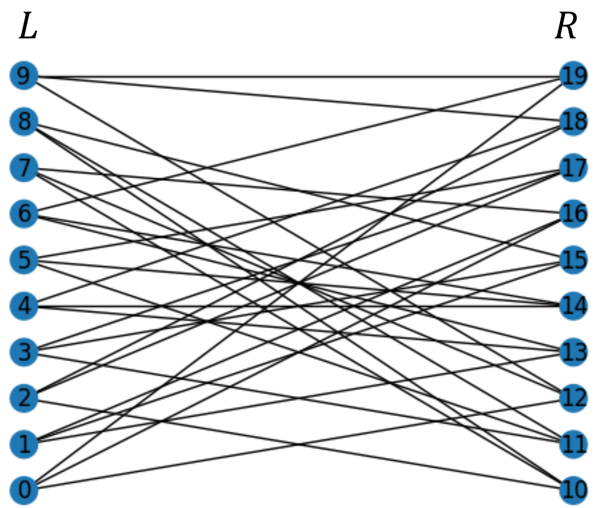
Then,

$$\mathcal{E}(\alpha, \beta) = \binom{n}{\alpha n}\binom{n}{\beta n}\left(\frac{\binom{(1-\beta)n}{\alpha n}}{\binom{n}{\alpha n}}\right)^{\Delta} = e^{\phi(\alpha,\beta)n(1+o(1))}$$

Consider the probability distribution μ over (α, β) induced by picking a random independent set in G. We have:

$$\mu(\alpha, \beta) \propto \mathcal{E}(\alpha, \beta) = e^{\phi(\alpha,\beta)n(1+o(1))}$$

→ μ corresponds to a Gibbs measure on (α, β) for the energy function ϕ and inverse temperature n



[DFJ02] M.Dyer, A.Frieze, M.Jerrum, "On counting independent sets in sparse graphs"

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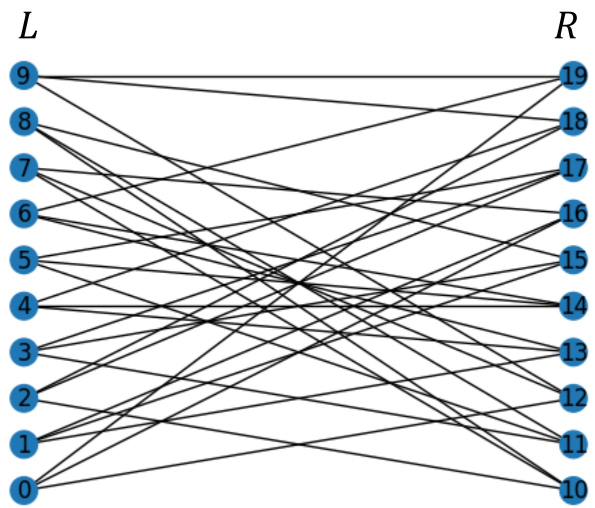
[DFJ02]: μ has exponential bottleneck when $\Delta \geq 6$.

Can we see this tendency quantumly?



Elie: Put (x, y)-plot?

- $\boldsymbol{\Delta \leq 4}$
- $\boldsymbol{\Delta \geq 6}$

[DFJ02] M.Dyer, A.Frieze, M.Jerrum, “On counting independent sets in sparse graphs”

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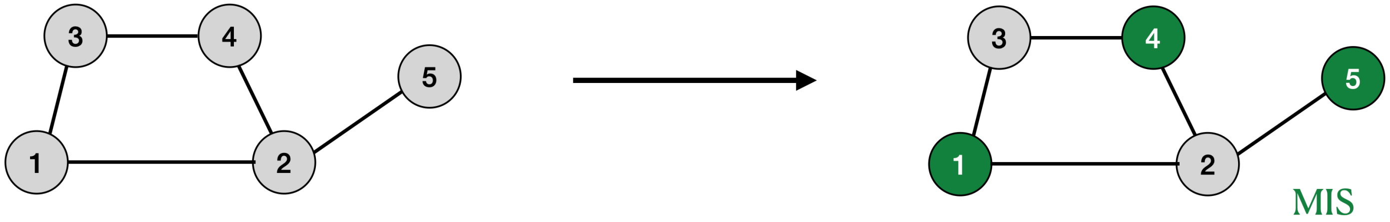
Quantum annealing and optimization



Each node has a label $n_i = \{0; 1\}$

Space of solutions $S = \{0; 1\}^N$ and $|S| = 2^N$

Associated cost function $C(n_1, \dots, n_N) = -\sum_{i=1}^{N} n_- + U \sum_{(i,j)\in E} n_i n_j$ with $U \gg 1$

We can encode in the ground-state of an Ising Hamiltonian the solution of the MIS

$$H_C = \sum_{i=1}^{N} \hat{n}_i + U \sum_{(i,j)\in E} \hat{n}_i \, \hat{n}_j$$

Such that

$$H_C |n_1, \dots, n_N\rangle = C(n_1, \dots, n_N) |n_1, \dots, n_N\rangle$$

<u>Goal</u>:Find the ground state of H_C

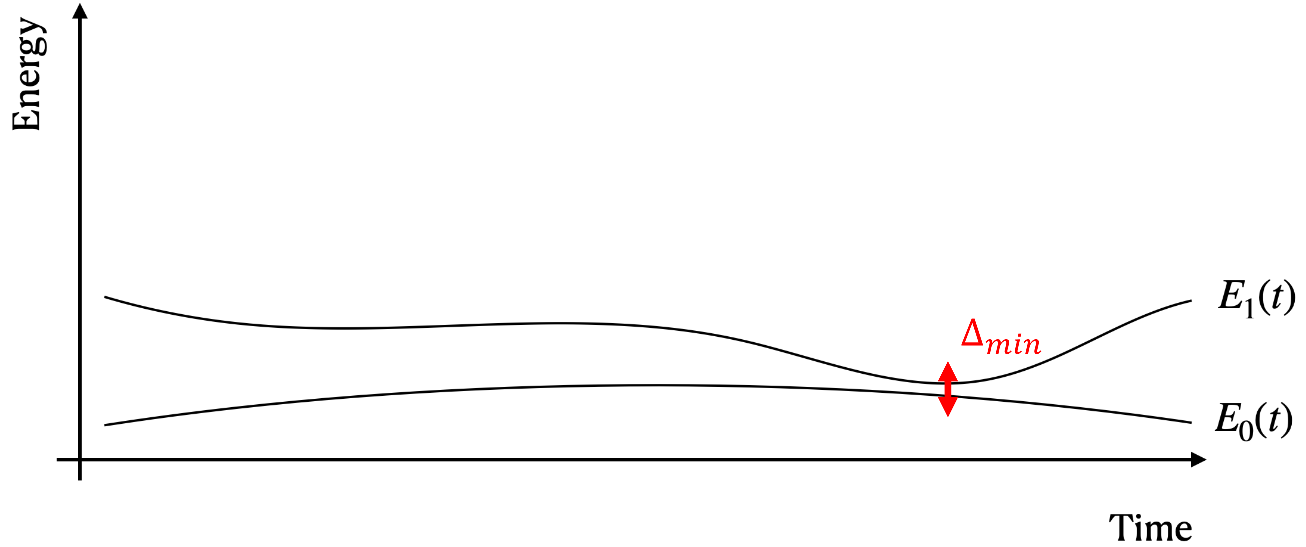
Quantum annealing and optimization

How do you actually "get" the ground state of $H_C \rightarrow$ Quantum adiabatic algorithm (QAA)

Step 1: Start from an "easy-to-prepare" ground-state $|\psi(0)\rangle = |+\rangle^{\otimes N}$, the ground state of $H_M = -\sum_{i=1}^{N} \hat{\sigma}_i^x$

Step 2: Evolve the state under $H(t) = (1-t)H_M + tH_C$, where $t \in [0;1]$.

Step 3: If the evolution is "slow" enough, then for all times t, the state $|\psi(t)\rangle$ is close to the instantaneous ground-state.



$$\Delta_{min} = \min_{t\in[0;1]} [E_1(t) - E_0(t)]$$

$$\boxed{\text{Evolution time } T \gg O(N\Delta_{min}^{-2})}$$

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Quantum annealing and optimization

Aim: Is the QAA efficient?

$$\boxed{\text{Evolution time } T \gg O(N\Delta_{min}^{-2})}$$

Good

$$\Delta_{min} = O\left(\frac{1}{poly(N)}\right)$$

Bad

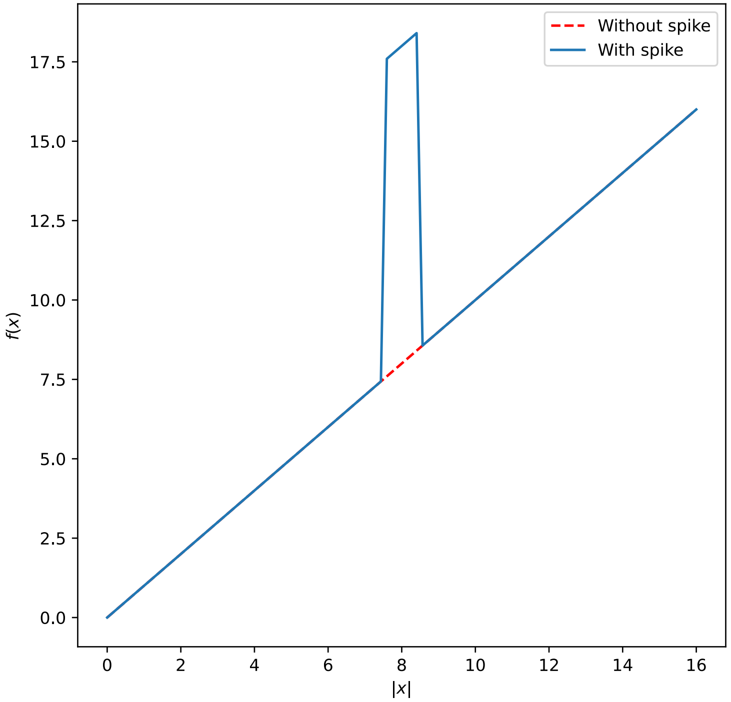
$$\Delta_{min} = O\left(\frac{1}{\exp N}\right)$$

Agenda

1	Introduction & Motivation
2	Quantum annealing and optimization for (M) IS preparation
3	Hamming weight with a spike problem
4	Independent set preparation
5	Conclusions and perspectives

Hamming weight with a spike [FGG02]

Problem: Find the minimum of a cost function perturbed with a spike e.g. $f(x) = |x| + h1(|x - B| \leq \eta)$



Ground state:

- Without spike $|\psi_0\rangle = |0..0\rangle$
- With spike $|\psi_0\rangle = |0..0\,\rangle$

Strategy: Optimization of quantum annealing

Result: Advantage of quantum annealing versus simulated annealing

[FGG02] E.Farhi, J.Goldstone, S.Gutmann "Quantum adiabatic evolution algorithms versus simulated annealing"

Hamming weight with a spike [FGG02] [Rei04]

Problem: Optimization of $f_h(x,y) = |x| + |y| + h1(\big||x| + |y| - B\big| \leq \eta)$ on pairs of states $(x,y) \in \{0;1\}^{2n}$

Strategy: Quantum adiabatic algorithm with Hamiltonians (and corresponding ground states)

$$H_M = -\sum_{i=1}^{2n} X_i \qquad |\psi_0\rangle = |+\rangle^{\otimes 2N} = \frac{1}{\sqrt{2^{2n}}} \sum_{(x,y)} |x,y\rangle$$

$$H_C(h) = \sum_{(x,y)\in\{0;1\}^{2n}} f_h(x,y)|x,y\rangle\langle x,y| \qquad |\psi_0\rangle = |0..0\rangle$$

Linear schedule $\qquad H(t,h) = (1-t)H_M + tH_C(h)$

Lemma: $\Delta(t) \coloneqq E_1(t) - E_0(t) \geq \sqrt{2} - \frac{h\eta}{\sqrt{n}}$

Elie: Put (x,y)-plot?

[FGG02] E.Farhi, J.Goldstone, S.Gutmann "Quantum adiabatic evolution algorithms versus simulated annealing"
[Rei04] B.W. Reichardt" The Quantum Adiabatic Optimization Algorithm and Local Minima"

Hamming weight with a spike [FGG02] [Rei04]

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Lemma: $\Delta(t) \coloneqq E_1(h,t) - E_0(h,t) \geq \sqrt{2} - \frac{h\eta}{\sqrt{n}}$

Idea of the proof:

- Get some results on the eigenstates/eigenvalues $(E_k(h,t), |\psi_k(h,t)\rangle)$ of $H(t,h) = (1-t)H_M + tH_C(h)$
- Solve the problem for $h = 0$ where we know the analytical solution $(E_k(0,s), |\psi_k(0,s)\rangle)$ [Rei04]
- Variational bound

$$E_0(h,t) - E_0(0,t) \leq \langle\psi_0(0,s)|H(t,h) - H(t,0)|\psi_0(0,s)\rangle$$

- Weyl's lemma $E_1(h,t) \geq E_1(0,t)$

Then, $\Delta(t) = E_1(h,t) - E_0(h,t) \geq E_1(0,t) - E_0(0,t) - \langle\psi_0(0,s)|H(t,h) - H(t,0)|\psi_0(0,s)\rangle$

Finally, $\langle\psi_0(0,s)|H(t,h) - H(t,0)|\psi_0(0,s)\rangle$ corresponds to an expectation value of a binomial distribution which can be easily bound.

[FGG02] E.Farhi, J.Goldstone, S.Gutmann "Quantum adiabatic evolution algorithms versus simulated annealing"
[Rei04] B.W. Reichardt" The Quantum Adiabatic Optimization Algorithm and Local Minima"

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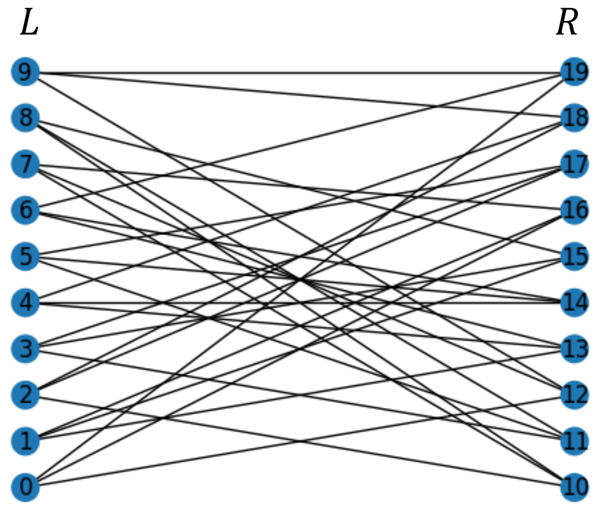
Quantum annealing for MIS

Problem: Optimization of $f(x,y) = -|x| - |y| + U\sum_{(i,j)\in E} x_i y_j$ on pairs of states $(x,y) \in \{0;1\}^{2n}$



Strategy: Quantum adiabatic algorithm:

$$H(t) = -(1-t)\sum_{i=1}^{2n} X_i + t\left(-\sum_{i=1}^{2n}\hat{n}_i + U\sum_{(i,j)\in E}\hat{n}_i\,\hat{n}_j\right)$$ with initial state $|\psi_0\rangle = |+\rangle^{\otimes 2N}$

Classically: The Gibbs measure looks like

$$\mu(\alpha,\beta) \propto \mathcal{E}(\alpha,\beta) = e^{\phi(\alpha,\beta)n(1+o(1))}$$

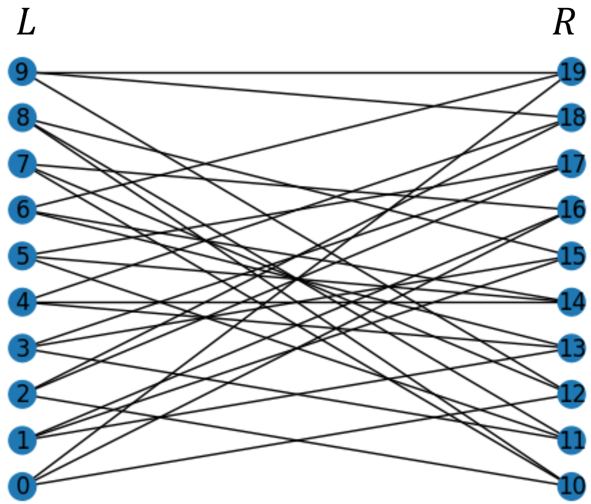
- [DFJ02] proved that $\phi(\alpha,\beta)$ has a single local maximum for $\Delta \leq 4$ and for $\Delta \geq 6, \phi$ has exactly two local maxima symmetrical (and an exponential bottleneck)
- Is it also the case for the probability distribution $p^t(z) = |a_z(t)|^2$ of the ground state $|\psi(t)\rangle = \sum_z a_z(t)|z\rangle$?

Elie: Put (x,y)-plot of $|\psi\ (t)\rangle$?
- $\Delta \leq 4$
- $\Delta \geq 6$

[DFJ02] M.Dyer, A.Frieze, M.Jerrum, “On counting independent sets in sparse graphs”

Quantum annealing for MIS - $\Delta \leq 4$

Problem: Optimization of $f(x,y) = -|x| - |y| + U\sum_{(i,j)\in E} x_i y_j$ on pairs of states $(x,y) \in \{0;1\}^{2n}$



Strategy: Quantum adiabatic algorithm:

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Observations:

- The potential $\phi(\alpha,\beta)$ has a single local maximum

Potential directions:

- Adiabatic algorithms without local maximum → Does it mean that our algorithm will converge with probability 1?
- Concentration/Cheeger inequalities for stoquastic Hamiltonians

Elie: Put (x,y)-plot of $|\psi(t)\rangle$?

- $\Delta \leq 4$
- $\Delta \geq 6$

[DFJ02] M.Dyer, A.Frieze, M.Jerrum, "On counting independent sets in sparse graphs"
[JP14] M.Jarret and S. P. Jordan, "Adiabatic optimization without local minima"

Quantum annealing for MIS - $\Delta \leq 4$

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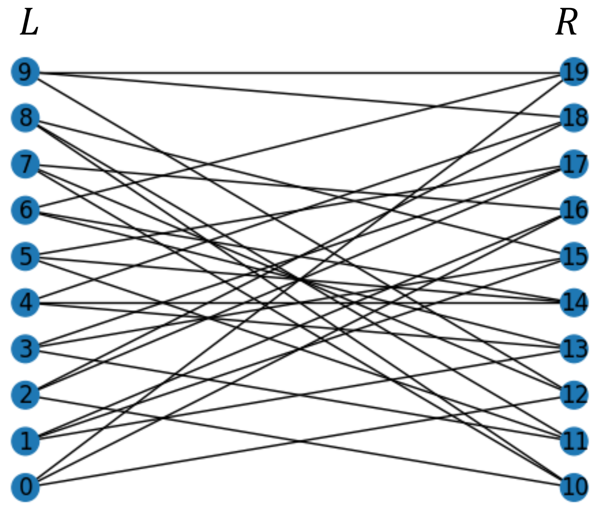

Strategy: Quantum adiabatic algorithm:

$$H(t) = -(1-t)\sum_{i=1}^{2n} X_i + t\left(-\sum_{i=1}^{2n}\hat{n}_i + U\sum_{(i,j)\in E}\hat{n}_i\,\hat{n}_j\right)$$ with initial state $|\psi_0\rangle = |+\rangle^{\otimes 2N}$

The potential $\phi(\alpha,\beta)$ has a single local maximum

Potential directions:

[JP14] proved that it implies that $\Delta(\mathrm{t}) \coloneqq E_1(t) - E_0(t) = \Omega\left(\frac{|W|^{-1}}{n^2}\right)$ with $|W| = \max_{(x,y)} f(x,y) - \min_{(x,y)} f(x,y) = Un^2 - n$ $(need\ to\ check\ that)$

Elie: Put (x,y)-plot of $|\psi\ (t)\rangle$?

- $\boldsymbol{\Delta \leq 4}$
- $\boldsymbol{\Delta \geq 6}$

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Conclusion

- Utilization of quantum annealing for combinatorial optimization problems like the MIS preparation
- Toy example of Hamming weight with a spike problem to prove polynomial advantage of quantum annealing versus simulated annealing method
- Current investigation of parallels between toy example and independent set preparations
  - Does the cost function of MIS preparation has similarities with the one of HW with a spike?
  - Can we prove some bottlenecks in the ground state probability distribution?
  - The quantum annealing Hamiltonian is stoquastic: $\forall x, y, \langle x|H(t)|y\rangle \leq 0$
    - Does it mean that we can prove a polynomial speedup?

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Appendix

Quantum case

Aim: Create a 2D-plot of (in)approximability for IS-sampling

Input: Let $G = (V, E)$ be an unbalanced bipartite graph with $V = L \cup R$, $|L| = \frac{n}{2}$ and $|R| = n$.

We construct this graph by taking the union of Δ L −perfect matching such that this graph has a maximum degree of Δ

Quantum annealing: $H(s) = -(1-s)(\sum_{i=1}^{\frac{n}{2}} \sigma_i^x + \sum_{\frac{n}{2}+1}^{\frac{3n}{2}} \sigma_i^x) + s\left(U \sum_{(i,j)\in E} n_i n_j\right)$

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Motivation

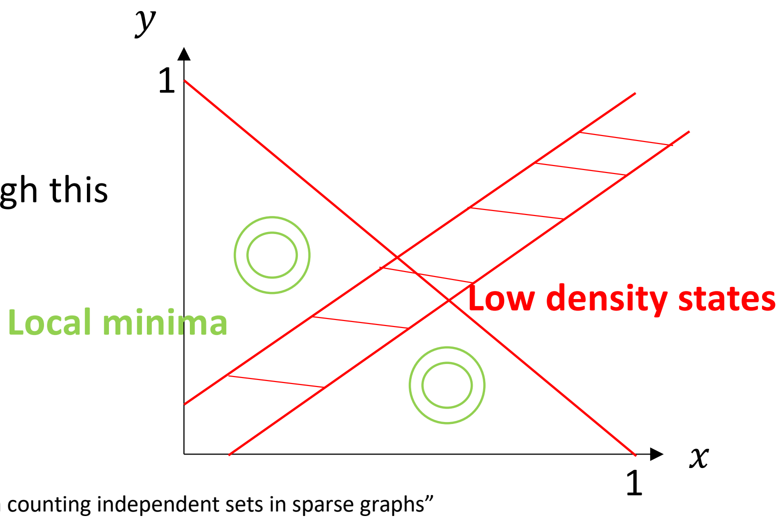
Method: We get $\mathbb{E}|\mathcal{I}(x,y)| = e^{\phi(x,y)n(1+o(1))}$
With $\phi(x,y) = -x\ln x - y\ln y - \Delta(1-x-y)\ln(1-x-y) + (\Delta-1)((1-x)\ln(1-x) + (1-y)\ln(1-y)$

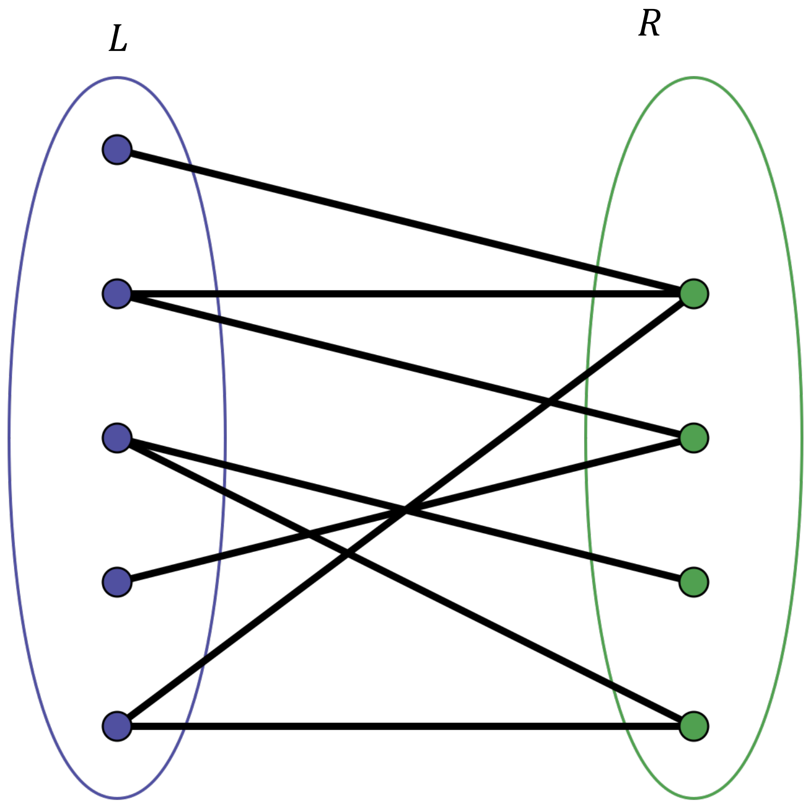
Define $\mathcal{T} = \{(x,y): x, y \geq 0 \text{ and } x+y \leq 1\}$, we have

- ϕ has no local minima in the interior of $\mathcal{T}$ and no local maxima on the boundary of $\mathcal{T}$
- All local maxima of ϕ satisfy $x + y + \Delta(\Delta-2)xy \leq 1$
- If $\Delta \leq 4$, ϕ has only a single local maximum which is on the line $x = y$
- If $\Delta \geq 6$, ϕ has exactly two local maxima symmetrical in x, y and a single

Saddle-point on $x = y$.

Aim: Can we go through this barrier quantumly?





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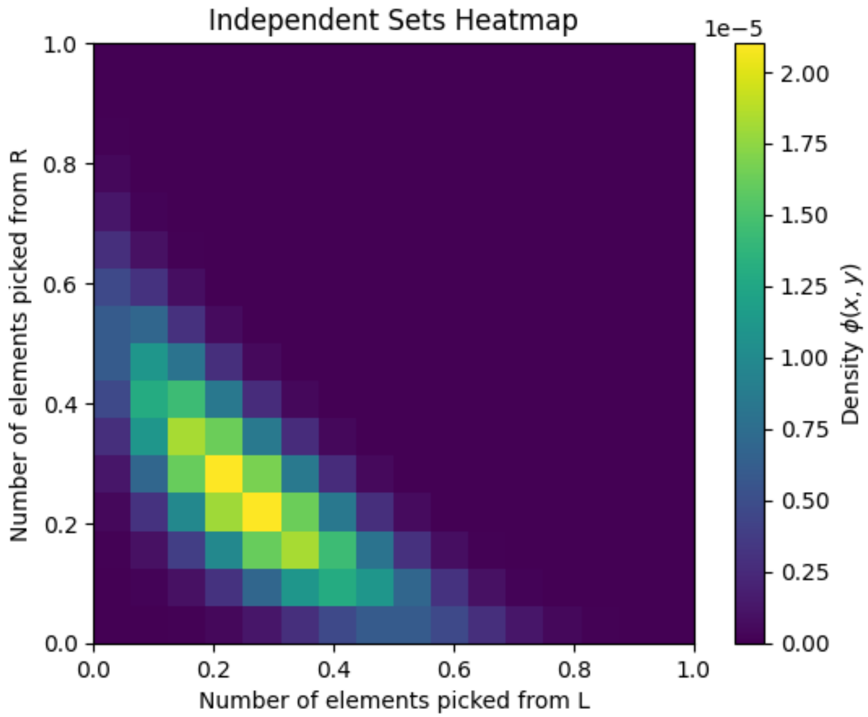
Motivation - Density $\phi(x, y)$

Example for size $N = 15$

$$d = 3$$



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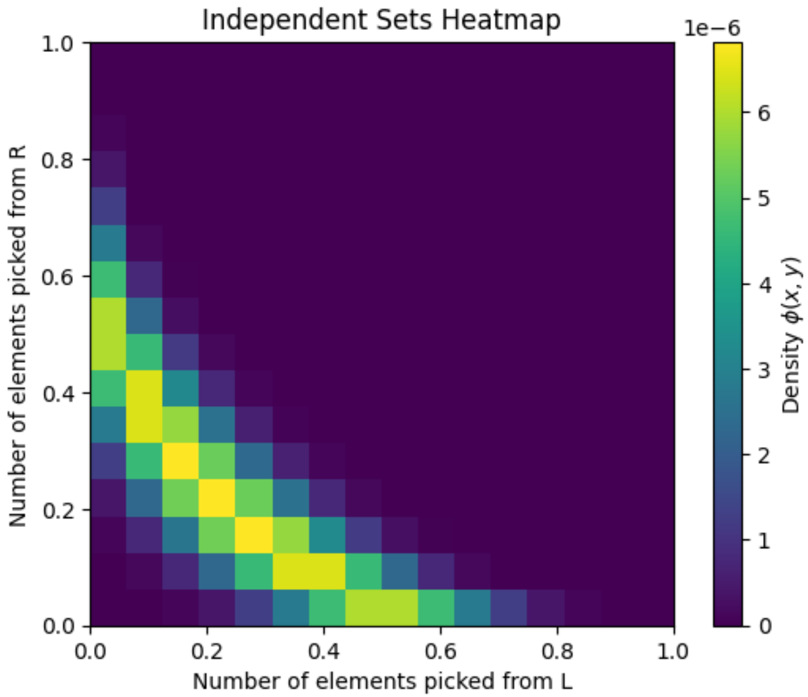
Motivation - Density $\phi(x, y)$

Example for size $N = 15$

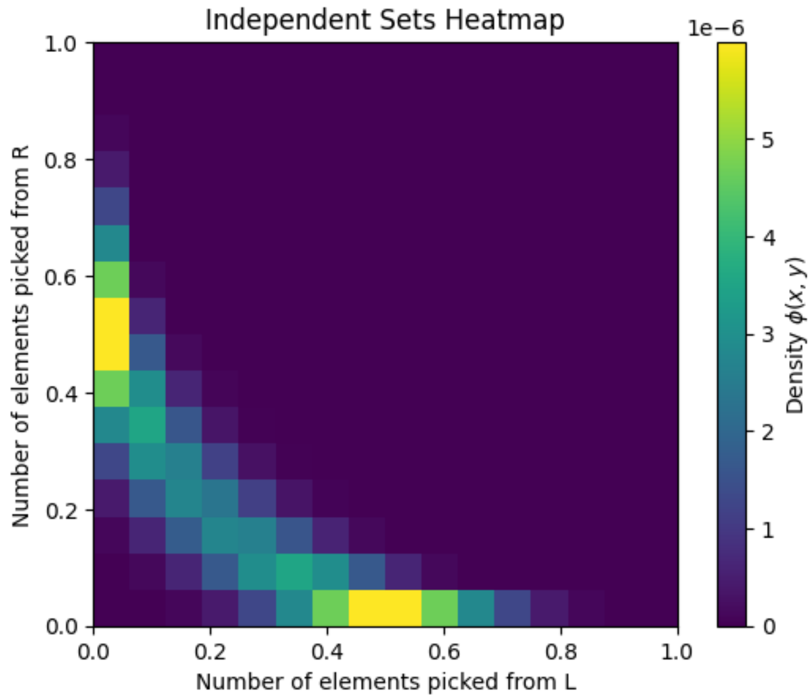
$$d = 4$$



Motivation - Density $\phi(x, y)$

Example for size $N = 15$

$$d = 5$$



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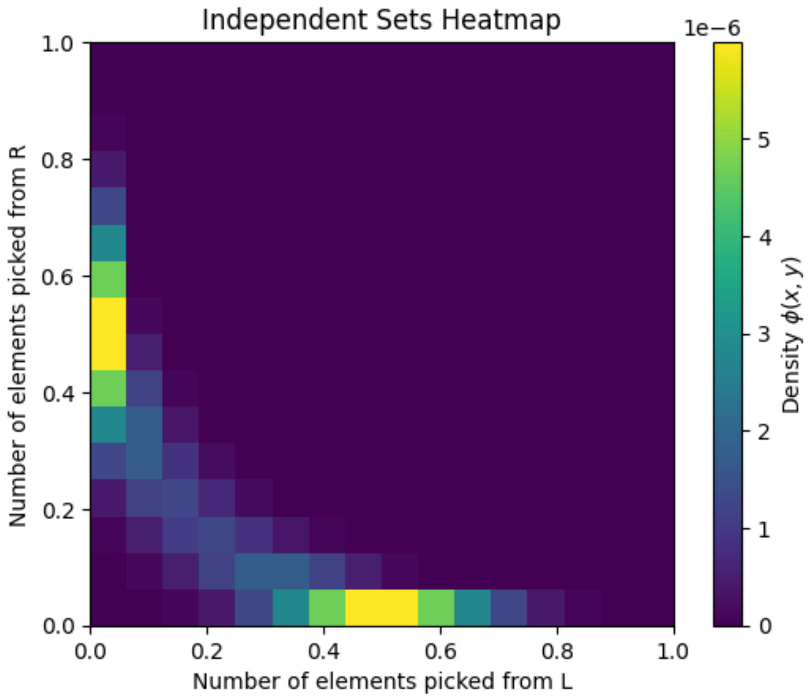
Motivation - Density $\phi(x, y)$

Example for size $N = 15$

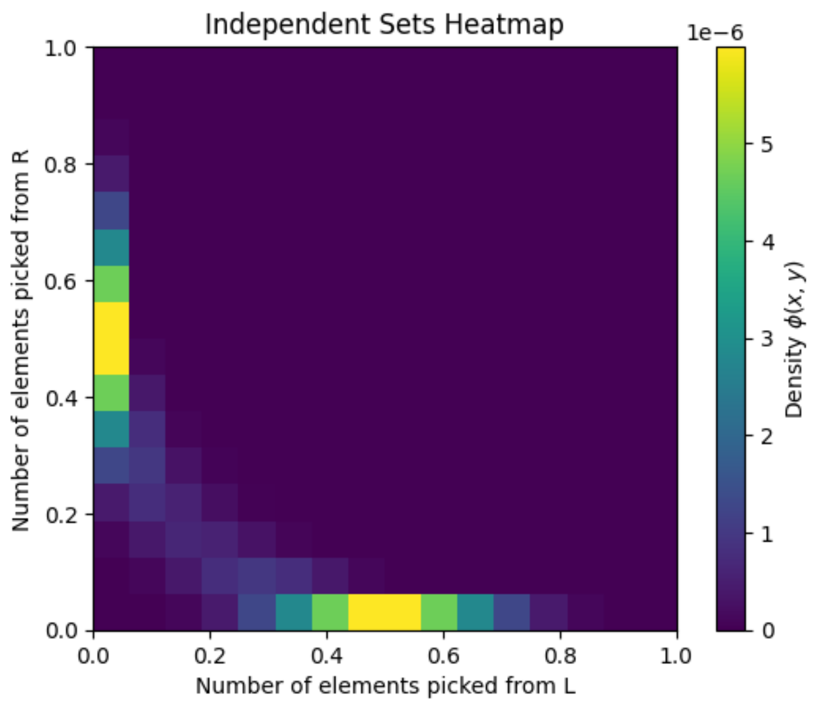
$$d = 6$$



Motivation - Density $\phi(x, y)$

Example for size $N = 15$

$$d = 7$$



Motivation – Unbalanced bipartite graphs

Method:

Let $G = (L \cup R,\ E), |L| < |R|$ (e.g. $|L| = \frac{n}{2}, |R| = n$

We define a L (resp. R) perfect matching as a set of disjoint edges which cover all edges of L (resp. R). By the marriage's theorem, this can happen iif for every subset W of$L$ (resp. R):

$$|W| \leq |N_G(W)|$$

with $N_G(W)$ the set of vertex of R that are adjacent to at least one element of$L$ (resp. R).
We pick a random graph by sampling Δ L-perfect matching. We consider that we generate independent sets from the sets $\mathcal{I}_{UB}(x,y)$ corresponding to sets $\sigma = V_1 \cup V_2$ with $|V_1| = \frac{xn}{2},\ |V_2| = yn$ and $V_1 \subset L, V_2 \subset R$

$$\begin{aligned}\mathbb{E}[|\mathcal{I}(x,y)|] &= |(choosing(x,y) - subsets)| \times \mathbb{P}[(x,y) - IS] \\ &= \binom{\frac{n}{2}}{\frac{xn}{2}} \binom{n}{yn} \left(\frac{\binom{(1-y)n}{\frac{xn}{2}}}{\binom{n}{\frac{xn}{2}}} \right)^{\Delta} \\ &= e^{\phi_{UB}(x,y)n(1+o(1))}\end{aligned}$$

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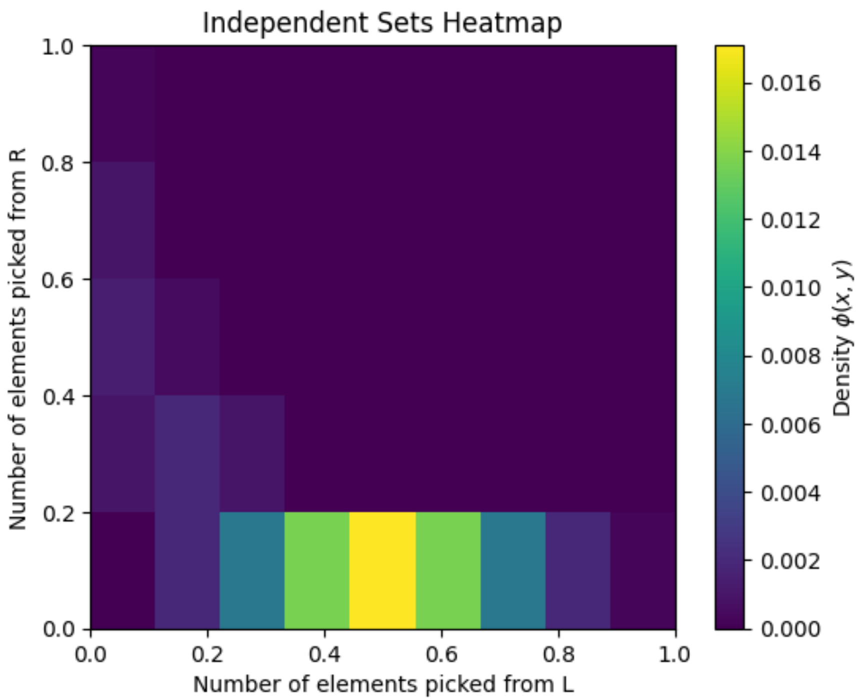
Unbalanced bipartite graphs

Example of an unbalanced bipartite graphs with $N = 14$



One local minima!

Quantum case

Aim: Create a 2D-plot of (in)approximability for IS-sampling

Quantum annealing: $H(s) = -(1-s)(\sum_{i=1}^{n} \sigma_i^x + \sum_{n+1}^{2n} \sigma_i^x) + sH_{IS}$, H_{IS} to be determined

Toy example: $H(s;h) = -(1-s)\sum_{i=1}^{2n} \sigma_i^x + s\,(\sum_{x,y\in(\{0,1\}^n)^2} \left(|x| + |y| + h1\big(\big||x| + |y| - B\big| \leq \eta\big)\right)|x,y\rangle\langle x,y|$ with eigenstates $\lambda_k(s,h), |\psi_k(s,h)\rangle$

$h = 0$:

- 2 non-interacting Hamiltonians $H(s,0) = -(1-s)(\sum_{1\leq i\leq n} \sigma_i^x + \sum_{n+1\leq i\leq 2n} \sigma_i^x) + s(\sum_{x\in\{0;1\}^n}(|x||x\rangle\langle x|) \otimes Id + Id \otimes \left(\sum_{y\in\{0;1\}^n}|y||y\rangle\langle y|\right)$
- Ground state $|\psi_0(s,0)\rangle = |v_1\rangle \otimes |v_2\rangle$
- All boils down to solve the 1-Hilbert case [1]

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Quantum case: 1 particule case and not interacting

$$p = \frac{(1-s)^2}{2\Delta(\Delta+s)}$$
$$q = \frac{(\Delta+s)^2}{2\Delta(\Delta+s)}$$

$H(s) = -(1-s)\sum_{1\le i\le n}\sigma_i^x + s\ \sum_{x\in\{0;1\}^n}|x||x\rangle\langle x|$: symmetry with Hamming weight

- Reduction from 2^n-dimensional Hilbert space to a $(n+1)$-one
- Basis states$|d\rangle = \frac{1}{\sqrt{\binom{n}{d}}}\sum_{x:|x|=d}|x\rangle, d = 0,..,n,$ in that subspace we have:

- $H(s) = (1-s)\sum_{i=0}^{n}(H_0)_i + s\ \sum_i (H_1)_i$ with $(H_0)_i = \frac{1}{2}\begin{pmatrix}1 & -1\\ -1 & 1\end{pmatrix}$ and $(H_1)_i = \begin{pmatrix}0 & 0\\ 0 & 1\end{pmatrix}$ thus corresponding to solving $(n+1)$ −non interacting spins with eigenstates on each subspace:
    - $E_{\mp} = \frac{1}{2}(1\mp\Delta)$, with $\Delta = \sqrt{1-2s+2s^2}$
    - $|a_{\mp}\rangle = \frac{1}{\sqrt{2\Delta(\Delta\pm s)}}(\pm(\Delta\pm s)|0\rangle + (1-s)|1\rangle)$
    - Thus, the ground state of $H(s)$ is $|v\rangle = |a_{-}\rangle^{\otimes n} = \frac{1}{(2\Delta(\Delta+s))^{\frac{n}{2}}}\sum_{x\in\{0;1\}^n}(1-s)^{|x|}(\Delta+s)^{n-|x|}|x\rangle = \sum_{0\le k\le n}\binom{n}{k}p^{\frac{k}{2}}q^{\frac{n-k}{2}}|k\rangle$
    - The eigenvalue gap Δ is minimized at $s = \frac{1}{2}$, when $\Delta = \frac{1}{\sqrt{2}}$

- Therefore, for our case of $h = 0$, $|\psi_0(s,0)\rangle = \frac{1}{(2\Delta(\Delta+s))^n}\sum_{x,y\in(\{0;1\}^n)^2}(1-s)^{|x|+|y|}(\Delta+s)^{2n-|x|-|y|}\ |x,y\rangle = \sum_{0\le k_1,k_2\le n}\binom{n}{k_1}\binom{n}{k_2}p^{\frac{k_1+k_2}{2}}q^{\frac{2n-k_1-k_2}{2}}|k_1\rangle|k_2\rangle$

with ground state energy $1-\Delta$ and the energy gap is 2Δ.

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Quantum case: Interacting case

$H(s;h) = -(1-s)\sum_{i=1}^{2n}\sigma_i^x + s\left(\sum_{x,y\in(\{0,1\}^n)^2}\left(|x|+|y|+h1\left(\big||x|+|y|-B\big|\leq\eta\right)\right)|x,y\rangle\langle x,y|\right.$ with eigenstates $\lambda_k(s,h), |\psi_k(s,h)\rangle$

$$p = \frac{(1-s)^2}{2\Delta(\Delta+s)}$$

$$q = \frac{(\Delta+s)^2}{2\Delta(\Delta+s)}$$

- $h=0, |\psi_0(s,0)\rangle = \frac{1}{\left(2\Delta(\Delta+s)\right)^n}\sum_{x,y\in(\{0;1\}^n)^2}(1-s)^{|x|+|y|}(\Delta+s)^{2n-|x|-|y|}\,|x,y\rangle = \sum_{0\leq k_1,k_2\leq n}\binom{n}{k_1}\binom{n}{k_2}p^{\frac{k_1+k_2}{2}}q^{\frac{2n-k_1-k_2}{2}}|k_1\rangle|k_2\rangle$

with ground state energy $1-\Delta$ and the energy gap is 2Δ.

- By monotonicity (Weyl's lemma) $\lambda_1(s,h)\geq\lambda_1(s,0)$
- We have $\lambda_0(s,h)-\lambda_0(s,0)\leq\langle\psi_0(s,0)|H(s,h)-H(s,0)|\psi(s,0)\rangle = sh\sum_{0\leq k_1,k_2\leq n}1(|k_1+k_2-B|\leq\eta)\binom{n}{k_1}\binom{n}{k_2}p^{k_1+k_2}q^{2n-k_1-k_2} = \mathbb{E}_{X,Y}[f(X,Y)]$

with $f(x,y) = 1(|x+y-B|\leq\eta)$,

- We have $\mathbb{E}_{X,Y}[f(X,Y)] = \mathbb{P}[|\mathrm{X}+\mathrm{Y}-\mathrm{B}|\leq\eta]$, with $X,Y\sim Bin(n,p)$, which means $Z\coloneqq X+Y\sim Bin(2n,p)$

We have $\mathbb{P}[|\mathrm{Z}-\mathrm{B}|\leq\eta]\leq\frac{\eta}{\sqrt{n}}$ (mostly because of how similar a binomial law and a normal distribution are+ binomial law has a width of about $\sqrt{m}$ when it is centered on strings of weight m

- Therefore, $\lambda_0(s,h)-\lambda_0(s,0)\leq\frac{hs\eta}{\sqrt{n}}\leq\frac{h\eta}{\sqrt{n}}$
- Then, $\lambda_1(s,h)-\lambda_0(s,h)\geq\lambda_1(s,0)-\lambda_0(s,h)\geq\lambda_1(s,0)-\lambda_0(s,0)-O\left(\frac{1}{\sqrt{n}}\right) = 2\Delta-\frac{h\eta}{\sqrt{n}}$
- We then have: $T\leq O\big(poly(n)\big)$

Tunneling works ✅

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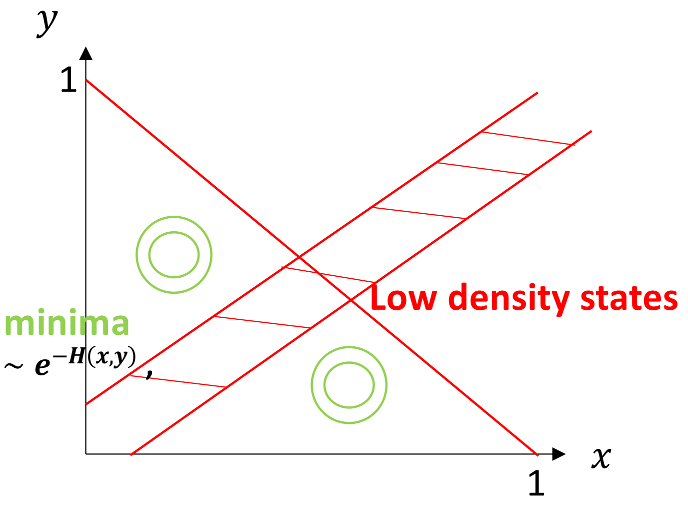
Next steps

<u>**Aim:**</u> Create a 2D-plot of (in)approximability for IS-sampling

Could we tunnel through this low-density barrier?

If we fix $x + y$ (i.e. the size of the IS), to what extend we can sample a random IS?



Density of states $\phi(x,y) = \mathbb{P}[(x,y) - partition\ is\ IS] \times \frac{|(x,y)partition|}{|partition|} = p(x,y)b(x,y) \sim e^{-H(x,y)}$,

$H(x,y) = -log\big(q(x,y)\big) = -log\big(Bin(x,y)\big) - \underbrace{log(p(x,y))}_{\text{perturbation}}$

Let's limit ourselves for now to one minimum, by making the bipartite graph unbalanced.

Application – Sample IS of size k

Aim: Create a 2D-plot of (in)approximability for IS-sampling

Input: Let $G = (V, E)$ be an unbalanced bipartite graph with $V = L \cup R$, $|L| = \frac{n}{2}$ and $|R| = n.$

We construct this graph by taking the union of Δ L −perfect matching such that this graph has a maximum degree of Δ

Quantum annealing: $H(s) = -(1-s)\sum_{1\leq i<j\leq n} S_{ij} + s\left(U\sum_{(i,j)\in E} n_i n_j\right)$ with $S_{ij} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}$ in the basis $\{ |00\rangle, |01\rangle, |10\rangle, |11\rangle\}$

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