Review

Fast quantum methods for optimization

S. Boixo[1], G. Ortiz[2] and R. Somma[3]

[1] Google Quantum A.I. Labs, Venice, CA 90291, USA
[2] Department of Physics, Indiana University, Bloomington, IN 47405, USA
[3] Theoretical Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

Abstract. Discrete combinatorial optimization consists in finding the optimal configuration that minimizes a given discrete objective function. An interpretation of such a function as the energy of a classical system allows us to reduce the optimization problem into the preparation of a low-temperature thermal state of the system. Motivated by the quantum annealing method, we present three strategies to prepare the low-temperature state that exploit quantum mechanics in remarkable ways. We focus on implementations without uncontrolled errors induced by the environment. This allows us to rigorously prove a quantum advantage. The first strategy uses a classical-to-quantum mapping, where the equilibrium properties of a classical system in d spatial dimensions can be determined from the ground state properties of a quantum system also in d spatial dimensions. We show how such a ground state can be prepared by means of quantum annealing, including quantum adiabatic evolutions. This mapping also allows us to unveil some fundamental relations between simulated and quantum annealing. The second strategy builds upon the first one and introduces a technique called spectral gap amplification to reduce the time required to prepare the same quantum state adiabatically. If implemented on a quantum device that exploits quantum coherence, this strategy leads to a quadratic improvement in complexity over the well-known bound of the classical simulated annealing method. The third strategy is not purely adiabatic; instead, it exploits diabatic processes between the low-energy states of the corresponding quantum system. For some problems it results in an exponential speedup (in the oracle model) over the best classical algorithms.

1 Introduction

Discrete combinatorial optimization problems are ubiquitous in science and technology but often hard to solve [1]. The main goal is to find the (optimal) configuration that corresponds to a global minimum of a given objective function. As the dimension of the search space typically grows exponentially with the size of the problem, finding the optimal configuration by exhaustive search rapidly becomes computationally intractable. This is the case even for relatively small problem sizes, specified by fifty or more bits. Efficient strategies for optimization are highly desirable.

Historically, some of the most practical optimization methods were developed in the context of physics simulation. Simulated annealing (SA) [2], for example, is a well-known method that imitates the cooling process of a classical system (e.g., a metal) that is initially heated and then cooled slowly, so that it ends up in one of the lowest-energy configurations. Ideally, the final state of the system is represented by the low-temperature Gibbs (equilibrium) distribution. To solve a combinatorial optimization problem with SA, the objective function is interpreted as the energy of the system. The annealing process can be simulated on a conventional (classical) computer by means of probabilistic Monte Carlo methods [3]. Such a process is determined by a sequence of transition rules, or stochastic matrices, that depend on a parameter associated with the (inverse) temperature of the system. In some cases, a good choice of transition rules allows us to sample an optimal configuration and solve the combinatorial optimization problem, with high probability, using significantly less resources than exhaustive search. SA can be applied to a variety of difficult problems, such as the well-known traveling salesman problem (TSP) [4] or Ising spin glasses [5].

Quantum mechanics provides remarkable tools for problem solving [6], and further motivates the search of novel and fast algorithms for optimization. A natural approach to develop such algorithms follows by considering a "quantum version" of SA. Rather than preparing a low-temperature Gibbs distribution of a classical system, the goal is now to prepare the lowest-energy or ground state of a *quantum* system. A projective measurement of the ground state would allow us to sample the optimal configurations, and solve the problem, with high probability. Such is the basic idea behind quantum annealing (QA) [7–9], adiabatic quantum computation (AQC) [10], or general quantum adiabatic state transformations [11]. These methods specify a quantum evolution to prepare the desired quantum state. The evolution can be simulated on a conventional computer by classical algorithms (e.g., by using quantum Monte Carlo methods or by numerical simulation of Schrödinger's differential equation) [12], on a quantum computer by quantum algorithms [11], implemented directly with quantum simulators (cf., [13]), or with programable physical QA architectures [14–16]. The complexity of each simulation or implementation may be different. The power of QA has been studied in a number of examples, such as in finding the low-energy configurations of Ising spin glasses [17,18].

This paper considers QA based methods for optimization and studies the complexity of such methods in the context of quantum computation or quantum simulation. Our QA strategies require a device that uses quantum coherence, such as a quantum computer or quantum simulator, for their implementation. Contrary to other results on the power of QA, which are commonly suggested from numerical evidence, our aim here is to mathematically prove that QA can outperform classical algorithms for some optimization problems. We will then focus in closed-system QA without uncontrolled errors induced by the environment, where the state of a quantum system generally evolves according to the Schrödinger equation, with the only condition that the final state is (close to) the appropriate eigenstate of the corresponding quantum system. In particular, AQC is one type of QA, with the additional constrain that the quantum evolution is adiabatic [19–24], so that the quantum state at any time is (close to) the ground state of the perturbed system[1]. A main goal of this paper is to theoretically and rigorously prove that *quantum implementations* of closed-system QA can be significantly more powerful than SA for solving optimization problems. In contrast, Refs. [14,16,18] study QA in the context of open-system dynamics.

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[1] Other continuous-time evolutions exploit diabatic transitions to prepare the ground state, such as those based on "shortcuts to adiabaticity" [25], and can be considered as a type of QA.

We study three different closed-system QA strategies. The first strategy considers a classical-to-quantum mapping, where a stochastic matrix is transformed into a Hamiltonian H_β that models a quantum system [26–28]. The ground state of this Hamiltonian is related to the stationary state of the stochastic matrix. That is, measurements of the ground state in the computational basis produces configurations according to the Gibbs distribution of the corresponding classical system. We then study the complexity of different QA techniques to prepare the ground state of H_β and compare it with the complexity of SA; QA and SA could have similar complexities in this case. The second strategy improves upon the first one and constructs a different Hamiltonian $\tilde{H}_\beta$ based on the idea of "spectral gap amplification" [29–31]. $\tilde{H}_\beta$ also has the ground state of H_β as eigenstate (not necessarily the ground state), so that QA can be used to prepare the eigenstate. We will prove that the complexity of preparing such a state, on a quantum device, is of order $1/\sqrt{\Delta}$, where Δ is a lower bound on the spectral gap of the stochastic matrix. This represents a quadratic quantum speedup with respect to SA, where the complexity is of order $1/\Delta$ [32]. (Typically, $\Delta \ll 1$ in hard instances of optimization problems.) The third strategy exploits diabatic transitions to excited states to prepare the ground state of the quantum system [33]. We show that this approach is efficient in solving a particular oracular problem [34], even though the minimum energy gaps are exponentially small in the problem size. In contrast, classical algorithms require (provable) exponential time in this case. We also discuss generalizations of this QA approach based on initial-state randomization to avoid some slowdowns due to small gaps, and comment on recent results on MAX 2-SAT, a NP-hard satisfiability (optimization) problem investigated in Ref. [35].

Each strategy is explained in detail in Sects. 2, 3, and 4, respectively. We summarize the results and conclude in Sect. 5.

2 Quantum vs. simulated annealing

Is QA fundamentally different from SA? Is there any reason why QA should outperform SA in solving optimization problems? In this section, we try to address these questions and explore some fundamental connections between SA and QA following Refs. [26–28, 30].

We first provide a short summary of the SA method for optimization. The search space of the combinatorial optimization problem, $\Sigma = \{\sigma_0, \ldots, \sigma_{N-1}\}$, consists of N configurations σ_i; the goal of SA is to find the (optimal) configuration that minimizes a given objective function $E: \Sigma \to \mathbb{R}$. Typically, each configuration σ_i can be associated with a state of a classical system defined on a lattice (or graph) Λ of size n, so that $E(\sigma_i)$ is the energy of the state. Each vertex of the lattice is a "site" of the classical system, and each site can be in one of M possible states. For example, if configurations are represented by n-bit strings (i.e., $N = 2^n$), the classical system may correspond to a classical Ising model of n sites, and $M = 2$. The spatial dimension of Λ is d.

Monte Carlo implementations of SA generate a stochastic sequence of configurations, via a sequence of Markov processes, that converges to the low-temperature Gibbs (probability) distribution defined by the probabilities

$$\pi_{\beta_m}(\sigma_i) \propto \exp(-\beta_m E(\sigma_i)). \tag{1}$$

When β_m is sufficiently large, sampling from the Gibbs distribution outputs the lowest-energy state of the system (i.e., an optimal configuration) with large probability. The annealing process is determined by a sequence of $N \times N$ stochastic matrices (transition rules) $S_{\beta_1}, S_{\beta_2}, \ldots, S_{\beta_m}$. The real parameters β_j denote a sequence of "inverse temperatures". If $|\beta_{k+1} - \beta_k|$ is sufficiently small, the annealing process drives

the Gibbs distribution from the initial $\beta_0 = 0$ (i.e., the uniform distribution) towards the Gibbs distribution for $\beta = \beta_m$ [32]. The stochastic matrices are chosen so that $\pi_\beta = (\pi_\beta(\sigma_0), \ldots, \pi_\beta(\sigma_{N-1}))^\mathsf{T}$ is the unique fixed point of S_β (i.e., $S_\beta \pi_\beta = \pi_\beta$), for all β. (T is the transpose.)

2.1 Classical-to-quantum mapping

Remarkably, any classical system on a lattice Λ can be related to a quantum system defined on the same lattice. To realize this "mapping", we associate each configuration or state σ_i with a quantum state $|\sigma_i\rangle$. Then, $\{|\sigma_0\rangle, \ldots, |\sigma_{N-1}\rangle\}$ forms a basis of a Hilbert space (i.e., the computational basis). In this basis, the objective function or energy functional E maps to a diagonal Hamiltonian matrix $\hat{E}$, where each diagonal entry is the corresponding $E(\sigma_i)$. For example, for classical Ising (spin-1/2) models, each configuration σ_i can be represented by the string $\sigma_i \equiv \sigma_i^0 \ldots \sigma_i^{n-1}$, where $\sigma_i^l = \pm 1$. Then, $\hat{E}$ can be written in operator form by replacing $\sigma_i^l \to \sigma_\mathbf{z}^l$ in E, where $\sigma_\mathbf{z}^l$ is the Pauli operator ($N \times N$ matrix) acting on the l-th site. For instance, quadratic objective functions are mapped to Ising models:

$$\hat{E} = \sum_{l=0}^{n-1} h_l \sigma_\mathbf{z}^l + \sum_{l,l'=0}^{n-1} J_{ll'} \sigma_\mathbf{z}^l \sigma_\mathbf{z}^{l'} , \tag{2}$$

where h_l denotes the local field of the spin at site l and $J_{ll'}$ denotes the Ising interactions between spins at sites l and l'.

In thermal equilibrium, the expectation value of a thermodynamic variable A in the canonical (Gibbs) ensemble is given by

$$\langle A \rangle_\beta = \mathcal{Z}_\beta^{-1} \sum_{\sigma_i \in \Sigma} e^{-\beta E(\sigma_i)} A(\sigma_i), \tag{3}$$

where $\mathcal{Z}_\beta = \sum_{\sigma_i \in \Sigma} e^{-\beta E(\sigma_i)}$ is the partition function. Note that $\pi_\beta(\sigma_i) = \mathcal{Z}_\beta^{-1} e^{-\beta E(\sigma_i)}$ is the Gibbs distribution and $\langle A \rangle_\beta = \sum_{\sigma_i \in \Sigma} \pi_\beta(\sigma_i) A(\sigma_i)$ is the corresponding average. The mapping between classical and quantum states also allows us to define $\hat{A}$, a diagonal $N \times N$ matrix or operator that has $A(\sigma_i)$ as diagonal entries. Then, we can rewrite Eq. (3) as

$$\langle A \rangle_\beta \equiv \langle \hat{A} \rangle_\beta = \langle \psi_\beta | \hat{A} | \psi_\beta \rangle, \tag{4}$$

where $|\psi_\beta\rangle$ is the (normalized) quantum state $|\psi_\beta\rangle = \sum_{\sigma_i \in \Sigma} \sqrt{\pi_\beta(\sigma_i)} |\sigma_i\rangle$. A projective quantum measurement of $|\sigma_i\rangle$ in $|\psi_\beta\rangle$ outputs the configuration σ_i with probability according to the Gibbs distribution.

The state $|\psi_\beta\rangle$ can be shown to be the unique ground state of certain quantum systems whose Hamiltonians are defined on the same lattice Λ [26–28,30,36–38]. Assume that the stochastic matrix S_β with unique fixed point π_β satisfies the "detailed balance condition" (DBC)

$$\Pr_\beta(\sigma_i | \sigma_j) \pi_\beta(\sigma_j) = \Pr_\beta(\sigma_j | \sigma_i) \pi_\beta(\sigma_i), \tag{5}$$

where $\Pr_\beta(\sigma_i | \sigma_j)$ is the conditional probability that specifies the (i, j) entry of S_β. Then, we define H_β via

$$\langle \sigma_i | H_\beta | \sigma_j \rangle = \delta_{i,j} - \sqrt{\Pr_\beta(\sigma_i | \sigma_j) \Pr_\beta(\sigma_j | \sigma_i)} . \tag{6}$$

Using the DBC, a simple analysis shows that $H_\beta \geq 0$ and $H_\beta|\psi_\beta\rangle = 0$ [26–28,30]. Furthermore, H_β is irreducible when S_β is, and $|\psi_\beta\rangle$ is the unique ground state of H_β in this case. The eigenvalues of H_β are $1 - \lambda_i$, where λ_i are the eigenvalues of S_β.

We now provide a specific construction for a Hamiltonian H_β, following Refs. [26–28,30], that provides insight into the connections between SA and QA – see Sect. 2.2. For illustrative purposes, we consider again the classical Ising model and map it to a quantum Ising (spin-1/2) model. For simplicity, we assume that S_β is obtained via a very similar process than that for the so-called Metropolis-Hastings algorithm (or Glauber dynamics). If σ_i and σ_j differ in a single position (spin flip), we choose

$$\Pr_\beta(\sigma_i|\sigma_j) = \chi \exp\{\beta[E(\sigma_i) - E(\sigma_j)]\}. \tag{7}$$

The constant of proportionality can be set to

$$\chi = \exp(-\beta\kappa)/n, \tag{8}$$

where $\kappa = \max_{i,j} |E(\sigma_i) - E(\sigma_j)|$, and the maximum is taken over those i, j such that σ_i and σ_j differ by a single spin flip. This choice guarantees that the conditional probabilities are properly bounded. If σ_i and σ_j differ in two or more positions,

$$\Pr_\beta(\sigma_i|\sigma_j) = 0. \tag{9}$$

Further, normalization implies

$$\Pr_\beta(\sigma_j|\sigma_j) = 1 - \sum_{\sigma_i \neq \sigma_j} \Pr_\beta(\sigma_i|\sigma_j). \tag{10}$$

The classical-to-quantum mapping of Eq. (6) gives

$$H_\beta = \sum_{l=0}^{n-1} \chi \exp(\beta\hat{E}^l) - \chi\,\sigma_\mathbf{x}^l, \tag{11}$$

where $\hat{E}^l$ is the diagonal matrix obtained as

$$\hat{E}^l = (\hat{E} - \sigma_\mathbf{x}^l\,\hat{E}\,\sigma_\mathbf{x}^l)/2, \tag{12}$$

and $\sigma_\mathbf{x}^l$ is the Pauli "spin-flip operator" at site l. That is,

$$\sigma_\mathbf{x}^l = \mathbb{1}_2 \otimes \cdots \otimes \mathbb{1}_2 \otimes \underbrace{\sigma_\mathbf{x}}_{l\text{-}th \text{ position}} \otimes \mathbb{1}_2 \cdots \otimes \mathbb{1}_2 \;,\; \sigma_\mathbf{x} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

and $\mathbb{1}_2$ is the 2×2 identity matrix. In other words, $\hat{E}^l$ includes only those terms in $\hat{E}$ that contain $\sigma_\mathbf{z}^l$; e.g., for Eq. (2),

$$\hat{E}^l = \sigma_\mathbf{z}^l \left(h_l + \sum_{l' \neq l} J_{ll'} \sigma_\mathbf{z}^{l'} \right). \tag{13}$$

Simple inspection shows that $(\exp(\beta\hat{E}^l) - \sigma_\mathbf{x}^l)|\psi_\beta\rangle = 0$ for all l, and $(\exp(\beta\hat{E}^l) - \sigma_\mathbf{x}^l) \geq 0$ [26]. These properties imply that H_β is a so-called "frustration-free Hamiltonian" – see Sect. 3. We remark that the range of interactions in H_β is determined by that of $\hat{E}^l$ or, equivalently, $\hat{E}$.

We emphasize the simplicity of Eq. (11): The thermodynamic properties of any finite two-level (spin-1/2) classical system at nonzero temperature can be obtained

by computing the ground state properties of a spin-1/2 quantum system, whose interactions depend on β and E, and an external and homogeneous transverse field. Remarkably, this field generates quantum fluctuations that are in one-to-one correspondence with the classical fluctuations at the inverse temperature β. In particular, $H_{\beta=0} = \mathbb{1}_{2^n} - \sum_{l=0}^{n-1} \sigma_{\mathbf{x}}^l/n$, thus its ground state has all spins aligned along the external field, i.e. $|\psi_{\beta=0}\rangle = \sum_{\sigma_i \in \Sigma} |\sigma_i\rangle/\sqrt{2^n}$. This quantum state can be identified with the completely mixed state (uniform distribution) of the classical model at infinite temperature. In general, the low-temperature limit is $|\psi_{\beta\to\infty}\rangle \to \sum_{\sigma_i \in \Sigma_0} |\sigma_i\rangle/\sqrt{|\Sigma_0|}$, where $\Sigma_0 \subseteq \Sigma$ is the set of optimal configurations or states that minimize E.

As shown in Ref. [26], the above classical-to-quantum mapping can be realized in any finite-dimensional classical system in addition to Ising-like (two states) or spin-1/2 models. In Ref. [26], we illustrated this generality by mapping a classical (three-state) Potts model into its corresponding quantum version on the same lattice.

2.2 State preparation and rates of convergence

The fact that $|\psi_\beta\rangle$ is the unique ground state of a simple Hamiltonian motivates the development of quantum methods to prepare it. The most natural methods in this context are those based on QA, including the recently developed methods for quantum adiabatic state transformations in Refs. [11,39], whose complexities can be shown to be smaller than that determined by standard adiabatic approximations (cf., [40,41]). Such methods require a quantum computer or simulator for their implementation.

Similar to SA, one QA method considers changing β slowly from $\beta_0 = 0$ to β_m in the Hamiltonian H_β of Eq. (6). In contrast to SA, this evolution is coherent and β does not correspond to the actual inverse temperature of the quantum system, which is assumed to be at zero temperature at all times (i.e., β is a parameter that determines the strengths of the interactions in the quantum system). If the system is closed and the evolution is adiabatic [19–24], the state of the system remains sufficiently *close* to the ground state $|\psi_\beta\rangle$ along the path, transforming $|\psi_{\beta_0}\rangle$ into the desired state $|\psi_{\beta_m}\rangle$. (Usually, $|\psi_{\beta_0}\rangle$ can be prepared easily.)

The total evolution time of the above QA method is determined by the quantum adiabatic approximation and depends on the spectral gap Δ_β of H_β, which is the difference between the two lowest eigenvalues of H_β (i.e., the first positive eigenvalue in this case). For arbitrary precision, such a gap determines a bound on the rate at which β can be increased. Assuming $E = O(n)$, which is typical in, e.g., Ising models, the gap satisfies $\Delta_\beta = \Omega(\exp(-\beta pn))$, where $p > 0$ is a constant [26]. This lower bound was determined using the inequalities in Ref. [42]. It is based on the worst-case scenario, so it is expected to be improved on a case-by-case basis by exploiting the structure of H_β (or S_β). According to the folk version of the quantum adiabatic approximation [19,20,26–28,30], the rate $\dot{\beta}(t)$ can be determined from

$$\frac{\|\partial_\beta|\psi_\beta\rangle\|\dot{\beta}(t)}{\Delta_{\beta(t)}} \leq \epsilon, \quad 0 \leq t \leq \mathcal{T}, \tag{14}$$

where ϵ is an upper bound to the error probability and $\mathcal{T}$ is the total time of the evolution. Note that $\|\partial_\beta|\psi_\beta\rangle\| \leq \|(\langle\hat{E}\rangle_\beta - \hat{E})|\psi_\beta\rangle/2\| \leq E_{\max}$, where $E_{\max} \geq \max_{\sigma_i} |E(\sigma_i)|$ is an upper bound on the objective function. Thus, $\|\partial_\beta|\psi_\beta\rangle\| = O(n)$ under the assumption on E.

In the limit $\log t \gg n \gg 1$, and for constant and small ϵ, integration of Eq. (14) with the bound $\Delta_\beta = \Omega(\exp(-\beta pn))$ gives

$$\beta(t) = O(\log t/n). \tag{15}$$

This result is somewhat similar to the Geman-Geman asymptotic convergence rate for SA obtained in Ref. [43]. Such an agreement results from the fact that Δ_β is also the gap of S_β (see Sect. 2.1), and the complexity of SA can be shown to be of order $1/\Delta_\beta$ [32].

The total evolution time can be determined from $\beta(\mathcal{T}) = \beta_m$. To obtain the optimal configuration with high probability from the Gibbs distribution, it suffices to choose $\beta_m = O(n)$ in the worst case. This gives a total time $\mathcal{T}$ or complexity for the current QA method (and similarly for SA) of order $\exp(c_1 n^2)$, for some constant $c_1 > 0$. This bound in complexity is larger than that of exhaustive search (which is exponential in n), but it is an absolute worst case bound and SA is performed much faster in practice. For example, in many cases it suffices to choose $\beta_m = O(\log n)$, leading to a $\mathcal{T} = \exp(c_2 n \log n)$, for some constant $c_2 > 0$.

As Eq. (14) does not necessarily constitute a necessary *and* sufficient condition for the validity of the adiabatic theorem [21–24], we explain next a version of the adiabatic approximation obtained by evolution randomization [39,44]. We discretize the path into m steps with separation $(\beta_{r+1} - \beta_r) = \Omega(1/n)$, and at the rth step we perform an evolution $e^{iH_{\beta_r}(\tau_1 + \tau_2)}$, with τ_i randomly chosen from the uniform distribution with support $[0, c_3 \Delta_\beta]$, for some constant $c_3 > 0$. Each random evolution effectively simulates a measurement of $|\psi_{\beta_r}\rangle$. Due to the quantum Zeno effect, this random process drives $|\psi_{\beta_0=0}\rangle$ towards $|\psi_{\beta_m}\rangle$, with high probability. The average cost of this method is

$$\langle \mathcal{T} \rangle = O(n^2/\Delta), \tag{16}$$

where Δ is a lower bound on $\min_\beta \Delta_\beta$, and we have used again the assumption $\beta_m = O(n)$, so that the total number of steps is $m = O(n^2)$. A bound for Δ_β gives a total cost analogous to that of the previous paragraph.

Another QA method to prepare the desired state, often used to find the ground states of Ising models, considers lowering a transverse field from a large initial value. In Ref. [9], the Hamiltonians are of the form $\hat{E} - \gamma \sum_{l=0}^{n-1} \sigma_\mathbf{x}^l$, where γ is the magnitude of a transverse field and $\hat{E}$ is the diagonal matrix that encodes the energies of the states of a classical Ising model (i.e., the objective function). This method can be modified to prepare $|\psi_{\beta_m}\rangle$, for $\beta_m < \infty$. To show this, we invoke the mapping of Eq. (6) and consider Eq. (11). Then, the Hamiltonians

$$H_\gamma = \sum_{l=0}^{n-1} \chi \exp(\beta_m \hat{E}^l) - \gamma \, \sigma_\mathbf{x}^l \tag{17}$$

can be used to prepare $|\psi_{\beta_m}\rangle$ on a quantum device by adiabatic state transformations, using a suitable $\gamma(t)$. The condition for the transverse field is $\gamma(\mathcal{T}) = \chi$, so that $H_{\gamma(\mathcal{T})} = H_{\beta_m}$ in that case, as in Eq. (11). In Refs. [26–28,30], we referred to this "finite-temperature" extension of the method of Ref. [9] as *Extended Quantum Annealing* (EQA). Note that, since the Hamiltonians in Eq. (17) do not suffer from the so-called sign problem, classical quantum Monte Carlo implementations of the EQA are also possible [30].

We use again the quantum adiabatic approximation to obtain a suitable $\gamma(t)$. To this end, we need a lower bound on Δ_γ, the spectral gap of H_γ. Considering the worst case instances and under the assumption $E = O(n)$, this gap satisfies $\Delta_\gamma = \Omega((\gamma/c_4)^n)$, for some $c_4 > \gamma$ [26]. The adiabatic approximation implies

$$\gamma(t) = O(t^{-1/(2n-1)}) \, . \tag{18}$$

Our result on the rate of change of γ coincides with that of Refs. [45,46]. The total evolution time $\mathcal{T}$ can be obtained from $\gamma(\mathcal{T}) = \chi$. Because $\chi = \exp(-\beta_m \kappa)/n$, the

scaling of the total evolution time as a function of β_m and n for the choice of Eq. (17) is the same as that of SA in Eq. (15).

We consider now the more standard QA method for Ising models mentioned above, where the Hamiltonians are of the form

$$\widehat{H}_\gamma = \hat{E} - \gamma(t) \sum_{l=0}^{n-1} \sigma_{\mathbf{x}}^l, \tag{19}$$

and the goal is to prepare the ground state of $\hat{E}$, as opposed to the Gibbs distribution for the inverse temperature β_m. The scaling result on the rate of change of $\gamma(t)$ found in Refs. [45,46] coincides with that of Eq. (18). There is no dependence on β when implemented in a quantum device as a closed system quantum evolution. The final value of the transverse field is $\gamma(\mathcal{T}) = O(1/n)$, which guarantees that the optimal configuration is found with high probability after measuring the ground state of $\widehat{H}_{\gamma(\mathcal{T})}$. This follows from perturbation theory, assuming that the spectral gap of $\hat{E}$ (i.e., the difference between the two smallest and different $E(\sigma_i)$) is $\Omega(1)$, i.e., bounded by a constant. The corresponding worst-case bound for the total evolution time is $\mathcal{T} = O(\exp(c_5 n \log n))$ in this case, for some constant $c_5 > 0$. This bound is still worse than that for the complexity of exhaustive search, but is better than the absolutely worst case bound obtained for SA resulting from Eq. (15), and analogous to the bound for SA corresponding to a low energy spectrum with a combinatorial number of elementary excitations. As remarked above, and similar to the results for SA, it is expected that in most practical cases much faster evolutions would suffice to solve the optimization problem.

Clearly, there are many Hamiltonian paths and corresponding methods that can be used to prepare $|\psi_{\beta_m}\rangle$ by means of QA. In the next section, we construct one such Hamiltonian path that yields a QA method to prepare the desired state with *provably* improved complexity than that given by the spectral gap bound for SA.

3 Spectral gap amplification

We show how to construct a Hamiltonian path with a spectral gap $\sqrt{\Delta_\beta}$ when given a SA algorithm where the stochastic matrices have a gap Δ_β. This will result in a quadratic quantum speedup for SA in terms of the spectral gap, which can be exponentially small in the problem size for hard instances of optimization problems. Our result is a generalization of Ref. [30], and the construction in this paper significantly simplifies the one used for Ref. [30]. We consider again the classical-to-quantum mapping of Eq. (6). When the DBC is satisfied by S_β, the Hamiltonian of Eq. (6) can also be decomposed as a "frustration-free" Hamiltonian. This decomposition will allow us to use the spectral gap amplification technique of Ref. [31][2].

For a Markov process with DBC, we define a corresponding undirected graph G as the graph with a vertex for each configuration and an edge for each pair

$$\left(\mathrm{Pr}_\beta(\sigma_i|\sigma_j), \mathrm{Pr}_\beta(\sigma_j|\sigma_i)\right). \tag{20}$$

For each edge we define an unnormalized state

$$|\mu_\beta^{(\sigma_i,\sigma_j)}\rangle = \sqrt{\mathrm{Pr}_\beta(\sigma_i|\sigma_j)}|\sigma_j\rangle - \sqrt{\mathrm{Pr}_\beta(\sigma_j|\sigma_i)}|\sigma_i\rangle. \tag{21}$$

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[2] For completeness, a Hamiltonian H is frustration free if it can be written as $H = \sum_k a_k \Pi_k$, with (known) $a_k \geq 0$, and $(\Pi_k)^2 = \Pi_k$ projectors. Further, if $|\psi\rangle$ is a ground state of H, then $\Pi_k|\psi\rangle = 0\ \forall k$. We assume $a_k \leq 1$.

Note that, from DBC, $\langle \mu_\beta^{(\sigma_i, \sigma_j)} | \psi_\beta \rangle = 0$. We also define the projection operators

$$O_\beta^{(\sigma_i, \sigma_j)} = |\mu_\beta^{(\sigma_i, \sigma_j)}\rangle \langle \mu_\beta^{(\sigma_i, \sigma_j)}|. \tag{22}$$

Then, Eq. (6) can be written as

$$H_\beta = \sum_{(\sigma_i, \sigma_j)} O_\beta^{(\sigma_i, \sigma_j)} \,. \tag{23}$$

This is a frustration free representation of H_β, as it is given by a sum of projectors, and each projector acts trivially on the ground state.

To apply the gap amplification technique of Ref. [31] efficiently, we need to reduce the number of operators in the frustration-free representation of H_β. [As is, the sum over σ_i, σ_j in Eq. (23) involves an exponentially large number of terms.] We can then assume a given edge coloring of the graph G with edge chromatic number q. It suffices to assume that the graph G has degree D, which gives a chromatic number at most $D+1 \geq q$ [47]. The degree D is determined by the stochastic matrix, as the edges of G are determined by the nonzero transition probabilities. For example, for the Glauber dynamics discussed in Sect. 2.1, $\Pr_\beta(\sigma_i | \sigma_j) \neq 0$ if both configurations differ by a single spin flip. Then, $D = n$ in this case. Let $z_1, \ldots, z_q$ be the different colors. All the operators $O_\beta^{(\sigma_i, \sigma_j)}$ belonging to one of the colors are, by construction, orthogonal to each other as they don't share a vertex. That is, $\mathrm{tr}[O_\beta^{(\sigma_i, \sigma_j)} O_\beta^{(\sigma_{i'}, \sigma_{j'})}] = 0$ for $i \neq i'$, $j \neq j'$. For each $k \in \{1, \ldots, q\}$, we define the Hermitian operators

$$O_{\beta,k} = \sum_{(\sigma_i, \sigma_j) \in z_k} O_\beta^{(\sigma_i, \sigma_j)}. \tag{24}$$

Then, $H_\beta = \sum_{k=1}^q O_{\beta,k}$ is a frustration-free representation. Note that there are many other ways to obtain a frustration-free representation, as the operators $O_\beta^{(\sigma_i, \sigma_j)}$ can be combined in several ways (i.e., other definitions for $O_{\beta,k}$ are possible).

Given a Hamiltonian H with ground state $|\psi\rangle$ and gap Δ, the goal of gap amplification is to find a new Hamiltonian $\tilde{H}$ with eigenstate $|\psi\rangle|\nu\rangle$ (not necessarily the ground state) and gap $\tilde{\Delta} > \Delta^{(1-\varepsilon)}$ with $\varepsilon > 0$. The state $|\nu\rangle$ is a fixed simple state. In addition, the implementation complexity of $e^{i\tilde{H}t}$ must be of the same order as the implementation complexity of e^{iHt}. The implementation complexity can be defined rigorously as the scaling of the number of quantum gates necessary to simulate this evolution in a universal quantum computer. This avoids trivial cases, like scaling the energies in H by a constant.

We now outline the gap amplification of H_β using a technique that applies to general frustration free Hamiltonians. We define the Hamiltonian

$$A_\beta = \sum_{k=1}^q \sqrt{O_{\beta,k}} \otimes (|k\rangle\langle 0| + |0\rangle\langle k|). \tag{25}$$

The first property to notice is that $\langle \psi_\beta 0 | A_\beta^\dagger A_\beta | \psi_\beta 0 \rangle = 0$ and $|\psi_\beta 0\rangle$ is an eigenstate in the null space of A_β.

We label the eigenvalues of H_β by λ_j, $j = 0, \ldots, N-1$, and $|\lambda_j\rangle$ are the eigenstates. We assume $\lambda_0 = 0 < \lambda_1 \leq \ldots \leq \lambda_{N-1}$, so that $|\psi_\beta\rangle = |\lambda_0\rangle$. Assume now $\lambda_j \neq 0$, and consider the action of A_β on the state $|\lambda_j 0\rangle$, that is,

$$A_\beta|\lambda_j 0\rangle = \sum_k \sqrt{O_{\beta,k}}|\lambda_j k\rangle. \tag{26}$$

Notice that

$$\langle\lambda_j 0|A_\beta|\lambda_j 0\rangle = \sum_k \langle\lambda_j k|\sqrt{O_{\beta,k}}|\lambda_j 0\rangle = 0, \tag{27}$$

and that

$$\|A_\beta|\lambda_j 0\rangle\|^2 = \sum_k \langle\lambda_j k|O_{\beta,k}|\lambda_j k\rangle = \lambda_j . \tag{28}$$

We denote by

$$|\perp_j\rangle = \frac{1}{\sqrt{\lambda_j}} A_\beta|\lambda_j 0\rangle \tag{29}$$

the corresponding normalized state. Next, note that

$$A_\beta|\perp_j\rangle = \frac{1}{\sqrt{\lambda_j}} \sum_k O_{\beta,k}|\lambda_j 0\rangle = \sqrt{\lambda_j}|\lambda_j 0\rangle . \tag{30}$$

Therefore, the Hamiltonian A_β is invariant in the subspace $\mathcal{V}_j = \{|\lambda_j 0\rangle, |\perp_j\rangle\}$. Define $(A_\beta)_j = (A_\beta)_{|\mathcal{V}_j}$ the projection of A_β in this invariant subspace. In the basis $\{|\lambda_j 0\rangle, |\perp_j\rangle\}$ we can write

$$(A_\beta)_j = \begin{pmatrix} 0 & \sqrt{\lambda_j} \\ \sqrt{\lambda_j} & 0 \end{pmatrix}, \tag{31}$$

with eigenvalues $\pm\sqrt{\lambda_j}$.

We note that, because the $|\lambda_j\rangle$ form a complete basis, A_β acts trivially on any other state orthogonal to $\oplus_j \mathcal{V}_j$, and therefore the eigenspace of eigenvalue 0 of A_β is degenerate. Although this step is unnecessary, we can avoid this degeneracy by introducing a "penalty term" to change the energies of the undesired eigenstates in such eigenspace. We then define the Hamiltonian

$$\tilde{H}_\beta = A_\beta + \sqrt{\Delta_\beta}(\mathbf{1} - |0\rangle\langle 0|). \tag{32}$$

The subspace orthogonal to $\oplus_j \mathcal{V}_j$ acquires eigenvalue $\sqrt{\Delta_\beta}$. Each space $\mathcal{V}_j$ is still an invariant subspace of $\tilde{H}_\beta$, and

$$(\tilde{H}_\beta)_j = \begin{pmatrix} 0 & \sqrt{\lambda_j} \\ \sqrt{\lambda_j} & \sqrt{\Delta_\beta} \end{pmatrix}. \tag{33}$$

The minimum eigenvalue of each of these operators is $\Omega(\sqrt{\Delta_\beta})$, which is also a bound on the relevant spectral gap of $\tilde{H}_\beta$[3].

For example, for the Hamiltonian H_β of Eq. (11), which is already expressed as a frustration-free Hamiltonian, we can write

$$\tilde{H}_\beta = \sum_{l=0}^{n-1} \sqrt{\chi\exp(\beta\hat{E}_l) - \chi\sigma_\mathbf{x}^l} \otimes (|l+1\rangle\langle 0| + |0\rangle\langle l+1|) + \sqrt{\Delta_\beta}(\mathbf{1} - |0\rangle\langle 0|). \tag{34}$$

In summary, the state $|\psi_\beta 0\rangle$ is generally the unique eigenstate of eigenvalue 0 of $\tilde{H}_\beta$. This eigenvalue is separated by a gap of order $\sqrt{\Delta_\beta}$. Also, the implementation complexity of evolutions with $\tilde{H}_\beta$ is similar to that of evolutions with H_β, under some

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[3] Note that the definition of $\tilde{H}_\beta$ depends on Δ_β, which is usually unknown. However, Δ_β can be replaced by its lower bound Δ in Eq. (32), still assuring a spectral gap of order $\sqrt{\Delta}$.
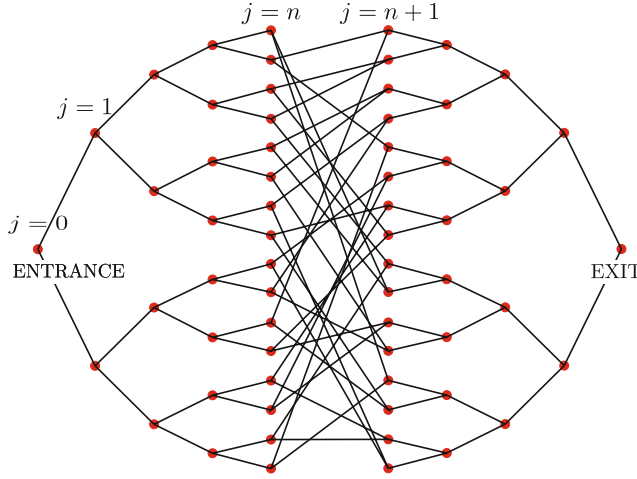
Fig. 1. (From [33].) Two binary trees of depth $n = 4$ glued randomly. The number of vertices is $N = 2^{n+2} - 2$. Each vertex is labeled with a randomly chosen $2n$-bit string. j is the column number.

reasonable assumptions. For the example of Eqs. (11) and (34), if $\hat{E}_l$ is a "local" operator that acts on a few spins, evolutions under H_β or $\tilde{H}_\beta$ can be efficiently implemented using known Trotter approximations or more efficient methods [48].

The implication of the spectral gap amplification technique is that the adiabatic approximation applied to prepare the (excited) state $|\psi_\beta 0\rangle$ results in a better scaling with Δ_β than in the case of H_β. To show this, we can use evolution randomization [39,44], which as explained in Sect. 2.2 is a rigorous version of the adiabatic approximation. The only change with respect to Sect. 2.2 is that the gap has been improved to $\sqrt{\Delta_\beta}$. This results in a quadratic speedup over SA with respect to the gap Δ_β, which is normally the dominating factor in the analytical bound for the cost of SA, as seen in Sect. 2.2. The dependence of $\langle \mathcal{T} \rangle$ on the error probability can be made fully logarithmic by repeated executions of the algorithm. We refer to Refs. [31,39,44] for more details about spectral gap amplification and evolution randomization.

To show that spectral gap amplification results in a provable quantum speedup, we can consider Grover's search problem. In this case, $E(\sigma_i) = 1$ for a particular, unknown σ_i, and $E(\sigma_j) = 0$ for all $\sigma_j \neq \sigma_i$. Classical algorithms to find σ_i have complexity $\Omega(N)$, i.e., they require evaluating the objective function in about half of the inputs, on average. It is possible to design a SA algorithm, whose stochastic matrices have gaps $\Delta_\beta = \Omega(1/N)$ to solve this problem. Then, spectral gap amplification results in a QA method that outputs σ_i, with high probability, and has complexity $O(\sqrt{N})$, improving quadratically upon the best classical algorithms.

4 Exponential speedup by quantum annealing

In this section, we first summarize our results in Ref. [33], where we considered the problem from Ref. [34] and solved it using QA. We are given an oracle that consists of the adjacency matrix A of two binary trees that are randomly "glued" (by a random cycle) as in Fig. 1. There are $N = O(2^n)$ vertices, which are named with randomly chosen $2n$-bit strings. The oracle outputs the names of the adjacent vertices on any given input vertex name. There are two special vertices, ENTRANCE and EXIT, the roots of the binary trees. They can be easily identified using A because they are the
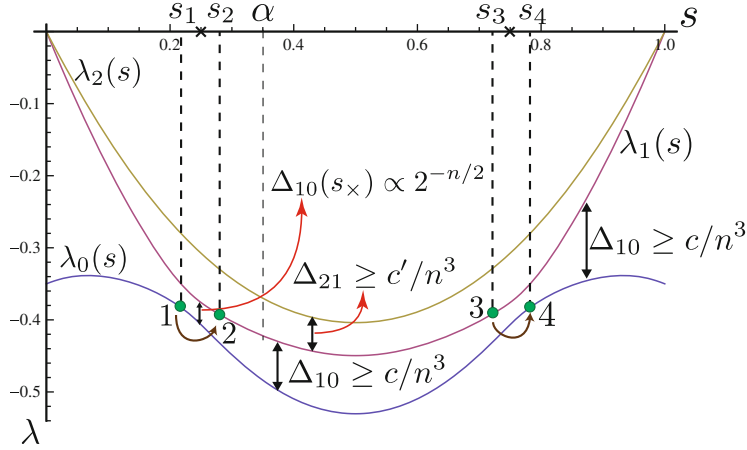
Fig. 2. (From [33].) Eigenvalues and energy gaps of $H(s)$, and scaling with the problem size n. $s_\times = \alpha/\sqrt{2}$ and $\alpha = 1/\sqrt{8}$ in this case.

only vertices of degree two in the graph. The glued-trees problem is: Given an oracle A for the graph and the name of the ENTRANCE, find the name of the EXIT. An efficient method based on quantum walks can solve this problem with constant probability, while no classical algorithm that uses less than a subexponential (in n) number of oracles exists [34]. Still, a direct QA method for this problem was unknown. We will then present a QA approach that efficiently outputs the name of the EXIT with arbitrarily high probability (in the asymptotic limit).

We let $a(V) \in \{0,1\}^{2n}$ be the bit string that labels vertex V. We assume a Hamiltonian version of the oracle so that evolutions under A can be implemented. Our Hamiltonian path for QA is given by ($0 \leq s \leq 1$)

$$H(s) = (1-s)H_{\text{ENTRANCE}} - s(1-s)A + sH_{\text{EXIT}}, \qquad (35)$$

with

$$H_{\text{ENTRANCE}}|a(\text{ENTRANCE})\rangle = -\alpha|a(\text{ENTRANCE})\rangle \,,$$

$$H_{\text{EXIT}}|a(\text{EXIT})\rangle = -\alpha|a(\text{EXIT})\rangle, \qquad (36)$$

and any other eigenvalues of these Hamiltonians are zero. $\alpha > 0$ is a constant, e.g., $\alpha = 1/\sqrt{8}$ works.

From Eq. (35), it is clear that when $s = 1$, the ground state of $H(1)$ is $|a(\text{EXIT})\rangle$. A measurement of this state allows us to obtain the solution to the glued-trees problem. The QA method is then designed to evolve the ground state of $H(0)$ towards that of $H(1)$. One may attempt to do this adiabatically. Nevertheless, the spectrum of $H(s)$, depicted in Fig. 2, shows that the smallest spectral gaps between the two lowest-energy states can be exponentially small in the problem size. This seems to imply that the total time required to adiabatically prepare $|a(\text{EXIT})\rangle$ from $|a(\text{ENTRANCE})\rangle$ would be exponentially large, resulting in an inefficient state preparation.

Remarkably, if s is changed in time so that it satisfies $\dot{s}(t) \propto 1/n^6$, the state $|a(\text{EXIT})\rangle$ can be prepared from $|a(\text{ENTRANCE})\rangle$ with arbitrary low error (in the asymptotic limit), thus solving the glued-trees problem efficiently. Such an annealing schedule for s implies that the initial ground state is eventually transformed into the first excited state for $s \geq s_\times$. But, at a later time, the symmetries of the spectrum around $s = 1/2$ imply that the first excited state is transformed back to the lowest-energy state (for $s \geq 1 - s_\times$), eventually preparing $|a(\text{EXIT})\rangle$ when $s \to 1$. The

evolution of the state is sketched in Fig. 2, where points (1,2) and (3,4) depict where the diabatic transitions between the two lowest-energy states occur. The details of the calculations for the spectral properties of $H(s)$, as well as the details about the efficient QA solution are given in Ref. [33].

It is important to note that, in the glued-trees problem, all the *interesting* quantum dynamics occurred in the manifold given by the two lowest-energy states. This additionally implies that, if when $s \to 0$ either state is prepared with probability $1/2$, the state $|a(\text{EXIT})\rangle$ would also be prepared with probability of almost $1/2$ by following an annealing schedule in which $\dot{s}(t) \propto 1/n^6$. The simple reasoning is that such a manifold is adiabatically decoupled from other excited states for that choice of $s(t)$. That is, the spectral gap between the first and second excited states, Δ_{21}, is of order $1/n^3$ rather than exponentially small for $1 > s > 0$– see Fig. 2. Thus, randomization of initial state preparation would also provide an efficient QA method to solve the glued trees problem, with probability of almost $1/2$.

One may wonder how general this efficient approach is for solving other optimization problems. Motivated by Ref. [33], in Ref. [35] the authors considered recently different QA evolutions to solve the well-known MAX 2-SAT problem. In this case, one is given a Boolean formula in conjunctive normal form, such that each clause contains at most two variables. The goal is two find an assignment to the variables such that a maximum number of clauses is satisfied. MAX 2-SAT is a NP-hard problem as one can reduce the well known NP-complete problem 3-SAT into MAX 2-SAT. The Hamiltonians used in the evolution act on a system of n qubits and are parametrized as $H(s) = (1-s)H_B + sH_P$ with

$$H_B = -\sum_{l=1}^{n} (1 - \sigma_\mathbf{x}^l)/2, \tag{37}$$

$$H_P = -\sum_{z \in \{0,1\}^n} f(z)|z\rangle\langle z|, \tag{38}$$

where $\sigma_\mathbf{x}^i$ is the Pauli spin flip operator acting on the lth qubit. $f(z)$ is the sum of the clauses in the Boolean formula on input z. Thus, a measurement on the ground state of H_P gives the solution to the corresponding MAX 2-SAT instance.

The ground state of H_P can be prepared using QA, evolving s from 0 to 1. The authors of Ref. [35] note that, for hard instances (according to a particular method that separates hard from easy instances) preparation of the ground state of H_P would take an extremely long time (simulations where ran for $n = 20$). Nevertheless, for those same instances, the probability of success in preparing the ground state is enhanced as one increases the rate of change of s. The nature of such an enhancement is similar to that of the glue-trees problem, where the QA evolution also generates diabatic transitions between different eigenstates. This opens a new door for the development of fast quantum algorithms, based on the idea of QA, for discrete optimization.

5 Conclusions

We presented three strategies to solve combinatorial optimization problems based on the idea of quantum annealing. All our strategies were developed in the context of quantum computation or quantum simulation, and will require a coherent quantum device for their implementation. Some strategies provide (provable) polynomial and exponential quantum speedups with respect to the corresponding classical methods for certain problems.

To obtain the results, we devised particular Hamiltonian paths and techniques so that the corresponding quantum evolution prepares a desired quantum state faster than the corresponding classical algorithm. First, we mapped the stochastic matrix of a classical Markov process into a quantum (frustration-free) Hamiltonian, whose ground state encodes the Gibbs (equilibrium) distribution of the classical system. In one case, we used the idea of spectral gap amplification, which is basically a mapping that takes a frustration-free Hamiltonian and efficiently outputs another Hamiltonian, having a much larger spectral gap, but preserving the ground state as eigenstate. A larger gap implied a (provable) faster way to prepare the desired quantum state adiabatically. In another case, we used the idea of diabatic transitions, allowing us to prepare a ground state by traversing other higher-energy states. Our techniques may be generalized to other problems; a step in this direction was recently given in Ref. [35].

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