A Framework for Structured Quantum Search

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Abstract

A quantum algorithm for general combinatorial search that uses the underlying structure of the search space to increase the probability of finding a solution is presented. This algorithm shows how coherent quantum systems can be matched to the underlying structure of abstract search spaces, and is analytically simpler than previous structured search methods. The algorithm is evaluated empirically with a variety of search problems, and shown to be particularly effective for searches with many constraints. Furthermore, the algorithm provides a simple framework for utilizing search heuristics. It also exhibits the same phase transition in search difficulty as found for sophisticated classical search methods, indicating it is effectively using the problem structure.

1 Introduction

Combinatorial search problems are among the most difficult computational problems because the time required to solve them often grows exponentially with the size of the problem [15]. Many such problems have a great deal of structure, allowing heuristic methods to greatly reduce the rate of exponential growth. Quantum computers [2, 3, 11, 12, 14, 25] offer a new possibility for utilizing this structure with quantum parallelism, i.e., the ability to operate simultaneously on a superposition of many classical states, and interference among different computational paths.

The physical restriction to unitary linear operations makes quantum computers difficult program effectively. Nevertheless, some algorithms have been developed. These include a method for efficiently factoring integers [33], a problem that appears to be intractable for classical computers. This method relies on rapidly identifying periods of periodic functions, so is limited to problems that can be cast in this form. More recently, a general search method was proposed [17]. While a substantial improvement over classical search for unstructured search spaces, it ignores the structure found in many combinatorial search problems thus limiting its effectiveness for such cases. In many such problems, solutions can be built incrementally from smaller parts, resulting in substantial improvement in classical searches through the use of heuristics that exploit this property. This observation forms the basis for a quantum search algorithm that uses structure in much the same way as classical heuristic searches [21].

These general search algorithms operate with superpositions of all possible search states for the problem. Each of their steps consists of adjusting the phases of the amplitudes in the superposition, based on properties of the problem being solved, combined with a problem-independent operation to mix amplitudes among different states. These algorithms are probabilistic and incomplete: they are likely to find solutions if any exist, but cannot guarantee no solutions exist. As with classical searches, the number of consistency tests (or checks) required by the algorithm characterizes search cost, although the detailed cost of each step will vary somewhat among different algorithms and implementations.
Specifically, the unstructured algorithm is likely to find one of \( S \) solutions among \( N \) possibilities with \( O(\sqrt{N/S}) \) checks \([3, 17]\). Without using additional structure, the fastest classical search is generate-and-test, where possible solutions are examined sequentially and which requires \( O(N/S) \) checks. Thus this quantum algorithm is a substantial improvement, and is close to the best possible for unstructured quantum searches \([5]\).

The structured algorithm \([21]\) builds solutions incrementally. Each trial requires only \( O(\log N) \) checks, but gives a low probability to find a solution, thus requiring multiple trials. The number of trials required is difficult to determine theoretically since the use of problem structure introduces many dependencies among the steps. Instead, as with many classical heuristic searches, the algorithm was evaluated empirically, which is necessarily limited to small problems due to the exponential slowdown associated with classical simulations of quantum computations. These simulations demonstrate a substantial improvement, on average, for classes of random problems.

While these algorithms are encouraging developments, the extent to which quantum searches can improve on heuristically guided classical methods for structured problems remains an open question. Even if quantum computers are not applicable to all combinatorial search problems, they may still be useful for many instances encountered in practice. This is an important distinction since typical instances of search problems are often much easier to solve than is suggested by worst case analyses, though even typical costs often grow exponentially on classical machines. The study of the average or typical behavior of search heuristics relies primarily on empirical evaluation. This is because the complicated conditional dependencies in search choices made by the heuristic often preclude a simple theoretical analysis, although phenomenological theories can give an approximate description of some generic behaviors \([20, 23, 29]\).

In fact, the hard instances are not only rare but also concentrated near abrupt transitions in problem behavior analogous to physical phase transitions \([6, 20, 19]\). These transitions correspond to a change from underconstrained to overconstrained problems and reflect changes in the structure of the problems. Problems located away from the transition region, i.e., with relatively few or relatively many constraints, tend to be easy to solve. These transitions appear with many classical search methods that use problem structure to guide choices, independent of the detailed nature of the search procedure. They thus reflect a universal property of classes of search problems rather than specific search algorithms. Similarly, the structured quantum algorithm also exhibits this transition. By contrast, the performance of unstructured search methods, such as generate-and-test and the unstructured quantum search algorithm, varies only with the number of solutions a problem has. Thus unstructured methods do not exhibit the transition, and in particular their search cost does not decrease when applied to increasingly constrained search problems. Thus an indication of whether a quantum algorithm exploits problem structure, through interference among different computational paths, is whether it exhibits the transition behavior.

In this paper, a new and analytically simpler structured quantum search algorithm is presented. Specifically the following two sections review the underlying structure of many combinatorial search problems and how structure can be used with quantum superpositions. The new algorithm is then described followed by an evaluation of its behavior. Finally some open issues are described. The structure-based algorithm provides a framework within which additional heuristics with knowledge of the structure of specific problems can be incorporated. It thus provides a way to develop and evaluate the use of heuristics for quantum searches, in a manner analogous to the use of heuristics to dramatically improve many classical search strategies.

## 2 The Structure of Combinatorial Search

NP search problems have exponentially many possible states and a procedure that quickly checks whether a given state is a solution \([15]\). Constraint satisfaction problems (CSPs) \([27]\) are an important example.
A CSP consists of $\nu$ variables, $V_1, \ldots, V_\nu$, and the requirement to assign a value to each variable to satisfy given constraints. Searches examine various assignments, which give values to some of the variables. Complete assignments have a value for every variable. Search states can also be viewed as sets of assumptions, where an assumption is an assignment to a single variable, e.g., $V_1 = 0$.

More generally, combinatorial search can be viewed as finding, from among $n$ given assumptions, a set of size $L$ satisfying specified constraints. Such a set is a solution to the problem. Sets of assumptions that violate a constraint are nogoods. In the particular case of CSPs, these include the necessary nogoods, in which some variables are assigned multiple values [37]. The remaining sets are goods, i.e., consistent. Supersets of a nogood are also nogood so sets of assumptions are usefully viewed as forming a lattice with levels from 0 to $n$, with level $i$ containing all sets of size $i$. This lattice, describing the consistency relationships among sets, is the deep structure of the combinatorial search problem. This structure for $n = 4$ is shown in Fig. 1. Notationally, we denote the size of a set $s$ by $|s|$.

![Figure 1: Set lattice for a problem with four assumptions, containing all subsets of \{1, 2, 3, 4\}. The bottom of the lattice, level 0, represents the single set of size zero, the four points at level 1 represent the four singleton subsets, etc.](image)

Classically, the necessary nogoods for CSPs can be avoided completely by searching only among assignments. Unfortunately, no quantum procedure can incrementally produce complete assignments from smaller ones with the variety of variable orderings needed for effective search [21]. Thus incremental quantum algorithms must use the expanded search space containing necessary nogoods.

This abstract description of combinatorial search in terms of sets of assumptions is less commonly used than other representations, which are more compact and efficient for classical search algorithms. It is introduced here as a useful basis for quantum searches and because it applies to many search problems, including CSPs.

Important examples of CSPs are graph coloring and satisfiability. In coloring an $\nu$-node graph with $c$ colors an assumption $V = \kappa$ is an assignment of a color $\kappa$ to a node $V$. Thus there are $n = \nu c$ assumptions.
for this problem and a solution is a set of $L = \nu$ such assumptions that gives a unique color to each node (i.e., contains no necessary nogood as a subset) and distinct colors to each pair of nodes in the graph that are linked by an edge. Each edge is a constraint directly specifying $c$ nogoods, each consisting of a pair of assumptions with the same color for both of the nodes linked by that edge. This search problem is known to be NP-complete for a fixed $c$ (at least equal to 3) as $\nu$ grows.

The satisfiability problem consists of a propositional formula in $\nu$ variables and the requirement to find a value (true or false) for each variable that makes the formula true. This problem has $n = 2\nu$ assumptions and $L = \nu$. An NP-complete example is 3-SAT, where the formula consists of a conjunction of clauses, and each clause is a disjunction of 3 of the variables in the problem, any of which may be negated. Thus a solution must satisfy every clause in the formula. An example of such a clause, with the third variable negated, is $V_1 \lor V_2 \lor \overline{V}_3$, which is false for exactly one assignment for these variables: \{\(V_1 = \text{false}, V_2 = \text{false}, V_3 = \text{true}\}\}. Thus each clause introduces a single nogood of size 3.

These examples show that challenging examples of combinatorial search occur when the nogoods directly determined by the constraints have a fixed size while the number of assumptions and the size of solutions grows linearly with problem size. This scaling, which gives a high concentration of hard instances [37], is used in the experiments described below.

## 3 Using Structure for Quantum Search

How can problem structure be used to improve quantum search? Some suggestions are provided by three categories of classical methods that use different aspects of problem structure. These methods contrast with unstructured searches, which amount to a random search among the states or a systematic enumeration of them without any use of prior results to guide future choices.

First, the problem can be simplified or abstracted in some way. A solution to the abstract problem is then used to guide the search in the original problem. If the abstract problem can be solved rapidly and its solution provides a good starting point for the full search, this strategy can be effective. For CSPs, abstraction can consist of ignoring some of the constraints or identifying useful hierarchical aggregations of variables and constraints.

A second method takes advantage of the clustering of solutions found in many search problems. That is, instead of being randomly distributed throughout the search space, the states have a simple neighborhood relationship such that states with a few or no conflicts tend to be near other such states. This neighborhood relationship is used by repair searches. Starting from a random state, they repeatedly select from among the current state’s neighbors one that reduces the number of conflicts with the constraints. Such searches can become stuck in local minima but are often very effective [28, 31]. More sophisticated versions address the problem of local minima by allowing occasional changes that increase the number of conflicts [22] as well as using a population of search states and combining parts from those with relatively few conflicts [10]. For example, with CSPs, the neighbors of a given complete assignment could be all other assignments with a different value for just one variable.

The third general search category builds solutions incrementally from smaller parts, which requires expanding the overall search space to include these smaller parts. These methods exploit the fact that in many problems the small parts can be tested for consistency before they are expanded to complete states. When a small state is found to be inconsistent, all possible extensions of it will also be inconsistent, allowing an early pruning of the search. In such cases, the search backtracks to a prior decision point to try a different incremental construction. For CSPs, this method assigns values to variables one at a time until a conflict is found. Its performance can be very good, but depends greatly on the choice of the order in which the variables are considered: a poor choice can mean few opportunities for early pruning.

In the context of quantum search, the general aspects of these methods could be used by a unitary
mapping that, at least approximately, maps amplitude from one state to others that would be considered after it by the corresponding classical method. In effect, this allows examining, and using interference from, all possible choices the classical search could have made, rather than being restricted to a single series of choices at a time. The details of the particular problem being solved could be introduced by adjustments to the phases of the amplitudes based on testing states for consistency. This technique, used with both the unstructured and structured quantum searches mentioned above, neatly separates the design of the unitary matrix that mixes amplitudes from any consideration of the detailed nature of specific problems. In particular, the structured algorithm builds solutions incrementally, but is difficult to analyze theoretically because the matrix elements used in the mapping procedure must be evaluated numerically. Thus it is of interest to see if there are analytically simpler structured methods that nevertheless retain the same properties of concentrating amplitude into solutions incrementally.

Toward this end we can consider the necessary size of the matrix elements connecting different sets. Consider the diffusion matrix used in the unstructured search algorithm [17]. Its off-diagonal terms have magnitude of size $O(1/N)$. If there is a single solution and we start from a uniform initial state with amplitudes $1/\sqrt{N}$, then even with a perfect choice of phases so each set gives a positive contribution to the solution, each step adds $O((1/N)N/\sqrt{N}) = O(1/\sqrt{N})$ to the solution set, because there are $N-1$ nonsolutions each mapped to the solution by a matrix element of size $O(1/N)$. Thus $O(\sqrt{N})$ steps will be required to give a solution amplitude of $O(1)$. This informal argument corresponds to that from a more detailed analysis of the unstructured algorithm [17, 5]. Starting with other initial conditions does not improve the situation, e.g., if all amplitude is initially in a single set, each step contributes $O(1/N)$ to the solution set, requiring $O(N)$ steps. Thus, any substantial improvement in search cost requires matrix elements with much larger couplings between sets. In particular, suppose each set receives substantial contributions from $z$ other sets with matrix elements of size $u$. Then normalization requires that $zu^2 \leq O(1)$. A single step, again assuming the phases are chosen perfectly, can transfer $O(uz/\sqrt{z}) = O(1)$ to a single set starting from a uniform distribution among the $z$ sets, or $O(u) = O(1/\sqrt{z})$ starting from all amplitude in a single set. This observation suggests that at least some matrix elements must be of size equal to a power of $O(1/\log N)$ to have a good chance of moving significant amplitude from one group of sets to a solution in a power of $O(\log N)$ steps. Such a matrix would be used to rapidly transfer amplitude from one group of sets to another, where each group is more likely to include solutions. Whether this performance can be realized depends on how well the phases can actually be chosen to give positive contribution to solutions and how the different groups of sets are selected. In the previous structured algorithm [21], and the new one presented below, these choices are based on searches that incrementally construct solutions from smaller parts.

4 A Structure-Based Quantum Search

A search with $n$ assumptions operates in the full lattice with $N = 2^n$ sets. Let $\psi_s^{(j)}$ be the amplitude of the set $s$ after completing step $j$ of the algorithm. A single trial of the search algorithm consists of:

1. initialize all amplitude in the empty set, i.e., $\psi_s^{(0)} = 1$ if the set $s = \emptyset$, and otherwise is zero.

2. iterate: for step $j$ from 1 to $J$, adjust phases based on consistency and then multiply by the matrix $U$ described below, to give

$$\psi_s^{(j)} = \sum_s U_{rs} \rho_s \psi_s^{(j-1)}$$

where $\rho_s$ is the phase assigned to the set $s$ as described below.

3. measure the final superposition
The phase adjustment is the only part of the algorithm that depends on the particular problem instance being solved. The choice of phase should move amplitude from nogoods to goods and also toward the largest goods, which are the solutions to the problem. In the previous structured and unstructured algorithms [17, 21], this phase choice consisted simply in inverting the phase of all nogoods, i.e., using $\rho_s = 1$ when $s$ is a good, and otherwise $\rho_s = -1$. This is an effective choice for the algorithm described here. However, performance is somewhat better in all but very highly constrained problems if, at each step, successively larger goods also have their phases inverted, i.e.,

$$\rho_s = \begin{cases} 
-1 & \text{if } s \text{ is nogood or } |s| < \min(L, j - 1) \\
1 & \text{otherwise}
\end{cases} \quad (2)$$

After $J$ steps, the final measurement gives a single set. This set will be a solution with probability

$$P_{\text{soln}} = \sum_s p(s) \quad (3)$$

with the sum over solution sets. Here $p(s) = |\psi_s^{(J)}|^2$ is the probability to obtain the set $s$ with the measurement of the final state. On average, the algorithm will need to be repeated $T = 1/P_{\text{soln}}$ times to find a solution.

The search cost can be characterized by the number of steps required to find a solution on average, i.e., $C = JT$. As described below, the matrix $U$ emphasizes mapping amplitude from sets to their supersets with one additional assumption. So one might expect the algorithm would require $L$ steps to give significant amplitude to sets of size $L$. However, the experiments reported below show fairly large amplitudes with somewhat fewer steps. In addition, instead of continuing the algorithm to maximize the probability to have a solution, a lower average search cost is sometimes possible by stopping earlier [5], a simple strategy for improving probabilistic algorithms [23]. Determining the best number of steps to take remains an open problem, but at worst one could try the algorithm for all values of $J$ up to $L$, resulting in at worst a linear increase in the overall search cost because $L \leq n$. More sophisticated methods for finding a suitable number of steps to take have been proposed for the unstructured search algorithm [5] and similar techniques may be useful for this structured search as well.

### 4.1 A Structure-Based Mapping

The matrix $U$, mixing amplitudes from different states, is the part of the algorithm that exploits structure to focus amplitude toward solutions. Specifically, let $U = WDW$ where, for sets $r$ and $s$,

$$W_{rs} = \frac{1}{\sqrt{N}} (-1)^{|r \cap s|} \quad (4)$$

and $D$ is a diagonal matrix of phases (complex numbers with magnitude equal to 1) depending only on the size of the sets, i.e., $D_{rr} = d_{|r|}$. The matrix $U$ is readily shown to be unitary and its multiplication of state vectors can be done rapidly on quantum computers using a recursive decomposition of the matrix $W$ [5, 17].

To take advantage of the lattice structure to incrementally construct solutions, the elements of $U$ mapping from a set to its supersets with one more item should be as large as possible. This can be done through appropriate choice of the values of $d_k$. Specifically,

$$U_{rs} = \frac{1}{N} \sum_{k=0}^{n} d_k S_k(r, s) \quad (5)$$
where

\[ S_k(r, s) = \sum_{t:|t|=k} (-1)^{|r \cap t| + |s \cap t|} \]  

(6)

with the sum over all sets \( t \) of size \( k \).

A given element \( e \) of \( t \) contributes 0, 1 or 2 to \(|r \cap t| + |s \cap t|\) when \( e \) is in neither \( r \) nor \( s \), in exactly one of \( r \) or \( s \), or in both \( r \) and \( s \), respectively. Thus \((-1)^{|r \cap t| + |s \cap t|}\) equals \((-1)^\lambda\) where \( \lambda \) is the number of elements in \( t \) that are in exactly one of \( r \) and \( s \). There are \((|r| - |r \cap s|) + (|s| - |r \cap s|)\) assumptions from which such elements of \( t \) can be selected. Thus the number of sets \( t \) of size \( k \) with \( \lambda \) elements in exactly one of \( r \) and \( s \) is given by \( \binom{m}{\lambda} \binom{n-m}{k-\lambda} \) where \( m = |r| + |s| - 2|r \cap s| \). Thus \( S_k(r, s) = S_{km}^{(n)} \) where

\[ S_{km}^{(n)} = \sum_{\lambda} (-1)^\lambda \binom{m}{\lambda} \binom{n-m}{k-\lambda} \]  

(7)

so that \( U_{rs} = \sum_k d_k S_{km}^{(n)}/N \equiv u_{m} \).

When \( s \) is an immediate subset of \( r \), i.e., \( s \subset r \) and \(|r| = |s| + 1\), we have \( m = 1 \). Thus the value of \( u_1 \) governs the mapping of amplitudes from sets to their immediate supersets and subsets. To select the values of \( d_k \) that maximize \( u_1 \), note that \( S_{01}^{(n)} = 1 \) and \( S_{11}^{(n)} = \binom{n-1}{k-1} \). Thus \( S_{k1}^{(n)} \) is positive for \( n > 2k \) and negative for \( n < 2k \), and \( u_1 \) is maximized by selecting \( d_k \) to be 1 for \( k < n/2 \) and -1 for \( k > n/2 \). If \( n \) is even, \( S_{k1}^{(n)} \) is zero for \( k = n/2 \) so the choice of \( d_{n/2} \) does not affect the value of \( u_1 \), though it does affect other matrix elements. In this case, we take \( d_{n/2} = 1 \). These choices give \( u_1 = \frac{2}{\sqrt{n}} \binom{n-1}{n/2} \) which scales as \( \sqrt{2/\pi n} \) as \( n \to \infty \). Note this is much larger than the off-diagonal matrix elements in the diffusion matrix used in the unstructured search algorithm [17], which are \( O(1/N) = O(2^{-n}) \). Unlike the previous structured search [21], \( U \) also gives some mixing among sets separated by more than one level in the lattice.

### 4.2 Classical Simulation

As a practical matter, it is helpful if a quantum search method can be evaluated effectively on existing classical computers. Unfortunately, the exponential slowdown and growth in memory required for such a simulation severely limits the size of feasible problems. For example, Eq. (1) is a matrix multiplication of a vector of size \( 2^n \) so a direct evaluation requires \( O(2^n) \) multiplications.

For the algorithm presented here, the cost of the classical simulation can be reduced substantially by exploiting the map’s simple structure. Specifically, the product \( WX \) can be computed recursively. To see this consider the sets ordered by the value of the integer with corresponding binary representation, e.g., the sets without item \( n \) come before those with \( n \). For example, the sets for \( n = 3 \) are ordered as \( \{\} \), \( \{1\} \), \( \{2\} \), \( \{1, 2\} \), \( \{3\} \), \( \{1, 3\} \), \( \{2, 3\} \) and \( \{1, 2, 3\} \). In this ordering, the matrix \( W \) has the recursive decomposition

\[ W = \begin{pmatrix} W' & W' \\ W' & -W' \end{pmatrix} \]  

(8)

where \( W' \) is the same matrix but defined on subsets of \{1, ..., \( n-1 \}\}. We can then compute

\[ WX = \begin{pmatrix} W'x^{(1)} + W'x^{(2)} \\ W'x^{(1)} - W'x^{(2)} \end{pmatrix} \]  

(9)

where \( x^{(1)} \) and \( x^{(2)} \) denote, respectively, the first and second halves of the vector \( x \) (i.e., corresponding to sets without \( n \) and with \( n \) respectively). Thus the cost to compute \( WX \) is \( C(n) = 2C(n-1) + O(2^n) \) resulting in an overall cost of order \( n2^n \). While still exponential, this improves substantially on the cost for the direct evaluation on classical machines.
5 Quantum Search Behavior

The behavior of this search algorithm was examined through a classical simulation. While these results are limited to small problems, they nevertheless give an indication of how this algorithm can dramatically focus amplitude into solutions. As a check on the numerical errors, the norm of the state vector remained within $10^{-10}$ of 1.

5.1 Extreme Cases

The simplest examples are the extreme cases of problems with the minimum and maximum possible number of nogoods. These cases have a very uniform consistency structure and may be particularly useful for analytic treatment of the algorithm. However, these problems are also rather easy for classical methods.

The minimum nogood problem consists of having all sets of size less than or equal to $L$ be goods, and all larger sets nogoods. Thus every set of size $L$ is a solution. Classical or quantum methods that operate only with complete sets (i.e., sets of size $L$) will find a solution in a single try. Classical incremental methods will require $L$ steps to construct a solution. Since $L = O(n)$, either type of search can solve this problem rapidly. For the structured quantum method, the amplitude of a set will depend only on the size of the set, i.e., $\psi_s = \psi_{|s|}$. Thus Eq. (5) becomes, for $h$ and $k$ running from 0 to $n$,

$$\psi_h^{(j+1)} = \sum_k V_{hk}^{\text{min}} \rho_k \psi_k^{(j)}$$

and Eq. (2) becomes $\rho_k = -1$ when either $k > L$ (i.e., the corresponding sets are nogood) or $k < \min(j - 1, L)$. The matrix in this mapping is $V_{hk}^{\text{min}} = W_{hk}^{\text{min}} D_{hk}^{\text{min}} W_{hk}^{\text{min}}$ where $D_{hk}^{\text{min}}$ is a diagonal matrix with $D_{kk}^{\text{min}}$ equal to 1 for $k \leq n/2$ and -1 otherwise, and

$$W_{hk}^{\text{min}} = \frac{1}{\sqrt{N}} \sum_z (-1)^z \binom{h}{z} \binom{n-h}{k-z} = \frac{S_h^{(n)}}{\sqrt{N}}$$

from Eq. (6). Here the binomials in the sum count, for a set $r$ of size $h$, the number of sets $s$ of size $k$ that have $z$ elements in common with $r$.

At the other extreme, the maximum nogood problem consists of having a single set of size $L$ and its subsets as goods and all other sets in the lattice as nogoods. This problem thus has a single solution, which without loss of generality we can take to be the set $\{1, \ldots, L\}$. In this case, search methods that operate with complete states will require more steps to find the single solution out of the total of $\binom{n}{L}$ complete states. However, the large number of nogoods will often allow classical heuristic repair methods to find a solution rapidly. Similarly, incremental classical methods will encounter conflicts immediately upon adding any assumption that is not a subset of the solution, thus allowing the solution to be found in $O(L)$ steps. For the structured quantum method, the amplitude of a set will depend only on the size of the set and its overlap with the single solution, i.e., $\psi_s = \psi_{|s|, |s| \cap \{1, \ldots, L\}}$. Hence the state can be represented by a doubly indexed vector $\psi_{kl}$ where $k$, giving the size of the set, ranges from 0 to $n$ and $l$, giving its overlap with the solution, ranges from $\max(0, k - (n - L))$ to $\min(k, L)$. Thus Eq. (5) becomes

$$\psi_{hj}^{(j+1)} = \sum_{kl} V_{hj,kl}^{\text{max}} \rho_{kl} \psi_{kl}^{(j)}$$

and Eq. (2) gives $\rho_{kl} = -1$ when either $k > L$ or $l < k$ (i.e., the corresponding sets are nogood) or $k < \min(j - 1, L)$. The matrix in this mapping is $V_{hk}^{\text{max}} = W_{hk}^{\text{max}} D_{hk}^{\text{max}} W_{hk}^{\text{max}}$ where $D_{hk}^{\text{max}}$ is a diagonal
matrix with $D_{kl,li}^\text{max}$ equal to $1$ for $k \leq n/2$ and $-1$ otherwise, and

$$W_{hj,kl}^\text{max} = \frac{1}{\sqrt{N}} \sum_{zx} (-1)^z \binom{L-j}{x} \binom{j}{l-x} \binom{h-j}{z-l+x} \binom{n-L-h+j}{k-z-x} \quad (13)$$

In this double sum, the binomials count, for a set $r$ of size $h$ with $j$ elements in common with the single solution, the number of sets $s$ of size $k$, with $l$ elements in the single solution, $z$ elements in common with $r$ and $x$ elements in the solution but not in the set $r$. This double sum separates to give

$$W_{hj,kl}^\text{max} = \frac{1}{\sqrt{N}} S_{h-j,k-l}^{(L)} S_{h-j,k-l}^{(n-L)} \quad (14)$$

from Eq. (13).

The scaling of the search cost for these extreme problems is shown in Fig. 2. The expected search cost grows quite slowly and is approximately a constant plus $n/4$ for both problems over the range of the figure. Furthermore, the optimal number of steps, i.e., the best value for $J$ in the algorithm also grows slowly. For the minimum nogoods problem, $J$ ranges from $2$ to $4$ over this range, while the maximum nogoods problem has $J$ ranging from about $5$ to $15$, and appears to grow as $O(\sqrt{n})$. In both problems, the best number of steps is considerably less than $L = n/2$. The slow growth in search cost for the maximum nogoods problem is particularly impressive since an unstructured quantum search requires of order $\sqrt{\binom{n}{L}}$ steps, which for $n = 100$ is about $3 \cdot 10^{14}$. As a final observation, if instead of Eq. (2), we just invert the phase of nogoods, the search cost is somewhat larger for the minimum nogoods problem, and somewhat lower for the maximum nogoods problem. Hence a variety of phase adjustment policies have good performance for these extreme problems.

![Figure 2](image_url)

Figure 2: Expected search cost for extreme problems for even values of $n$ with $L = n/2$. Black and gray curves are for problems with the maximum and minimum number of nogoods, respectively.

Further insight into the behavior of this algorithm is given by Fig. 3 which shows how the probability to have a good of different sizes varies with each step of Eq. (13). Specifically, for each step $j$ and each set
size $k$, the figure shows the value of $\sum_s |\psi_s^{(J)}|^2$ where the sum is over all good sets $s$ of size $k$. Since the size of goods is at most 50, the plot does not include larger sets. The initial condition (not shown) has probability 1 in the set of size 0. The algorithm maintains a concentration of amplitude in goods, and moves rapidly up the lattice to give a relatively large amplitude in the solution after 15 steps, considerably fewer than $L = 50$.

5.2 Intermediate Cases: Hard Problems

The difficult search problems, on average, have an intermediate number of constraints: not so few that most complete states are solutions, nor so many that any incorrect search choices can be quickly pruned.

Two examples of how the algorithm concentrates amplitude into solutions are shown in Fig. 4. For each problem, the figure shows the values of $|\psi_s^{(J)}|^2$ for each of the $2^n$ sets in the lattice. The solutions are drawn as gray points to distinguish them from the remaining sets. For the plots, the sets are ordered according to the integer whose binary representation corresponds to including the items in the set. For both of these problems, the lowest expected search cost is with $J = 5$, providing another illustration of the algorithm moving significant amplitude to the solution level of the lattice in fewer than $L$ steps.

In these problems, the constraints are specified by nogood assignments of size 2, corresponding to CSPs, such as graph coloring, where each constraint involves two variables. The value of $m$ denotes the number of such nogoods in the problem. These two examples illustrate the typical behavior for a problem with relatively few constraints, and many solutions, and a problem with many constraints and only one solution. There are $\binom{12}{6} = 924$ sets at the solution level, so a random selection would give a probability of about 0.001 to each set, much less than given to solutions by this algorithm. Thus the various contributions to nonsolutions tend to cancel out among the many paths through the lattice. The figure also illustrates the variation in $|\psi_s^{(J)}|^2$ among the sets showing that, unlike the extreme problems of the previous section, the amplitudes do not depend only on the size of the set and overlap with solutions. Rather the details of which constraints apply to each set give rise to the variation in values seen here.
This variation precludes a simple theoretical analysis of the algorithm.

### 5.2.1 Phase Transition

For a more general indication of how this algorithm uses the structure of search problems, we consider its average behavior for ensembles of problems with different degrees of constraint. One such ensemble consists of randomly generated instances of CSPs where the constraints specify $m$ nogoods of size 2 and $L = n/2$. Increasing $m$ changes the ensemble from weakly constrained to highly constrained problems, thus showing how the performance depends on the tightness of the constraints. Since the quantum algorithm can find solutions but never definitely prove that no solution exists, we examine only problems with at least one solution.

Specifically, for given values of $n$ and $m$, problem instances are generated as follows. First, we randomly select a complete assignment to be a solution for the problem. Then, from among the assignments of size 2 that are not subsets of this prespecified solution, we pick $m$ distinct sets to be the nogoods directly determined from the problem’s constraints. All these problems also have necessary nogoods to constrain each variable to have a unique solution. This generation procedure guarantees the problem has at least one solution since it never selects any subset of the prespecified solution to be a nogood.

Among the $\binom{n}{2}$ sets of size 2, $4\binom{L}{2}$ are assignments and the remainder are necessary nogoods. Of these assignments, $\binom{L}{2}$ are subsets of the prespecified solution. The remaining sets are available to be selected as the $m$ nogoods from the constraints. Thus to span the range from unconstrained to fully constrained problems, we can select $m$ to range from 0 to

$$m_{\text{max}} = 3\binom{L}{2}$$

The average behavior of the algorithm for these problem ensembles as the number of constraints are changed is shown in Fig. 5. This search algorithm exhibits the phase transition behavior described above as occurring for many classical searches [6]. Thus the algorithm is using interference of paths to exploit problem structure in the same manner as sophisticated classical search methods are observed to do.

Because the location of the transition is at a value of $m$ that grows linearly with $n$, the figure shows the search cost as a function of $\alpha = m/n$. More precisely, a mean-field theory of this behavior predicts
Figure 5: Average search cost $C$ as a function of $\alpha = m/n$ for $n = 16$ and 20 (black and gray curves, respectively). Each point is the average of 1000 problem instances, and includes error bars indicating the standard error of the mean, which are smaller than the size of the plotted points.

the the transition point, and the peak in the search cost, occur at $\alpha_{\text{crit}} = -\ln(2)/(2\ln(3/4)) = 1.2$ when $n$ is large [37]. For the quantum search, the figure shows the search cost peak is close to this value even for relatively small values of $n$.

A significant observation from Fig. 5 is that the quantum algorithm’s search cost decreases after the transition. By contrast, since the expected number of solutions continues to decrease as problems become more constrained, unstructured search methods do not show this decrease in cost. Thus the use of problem structure is relatively more beneficial for problems with many constraints.

As with other examples of phase transitions in search, the variance in search cost among different problems in the ensemble is relatively large near the transition point. Thus an interesting open question, for both classical and quantum search methods, is whether there are simple ways to identify those problems likely to be much harder or easier than the average. If these cases correspond to particular types of structure [36], it may be possible to develop specialized variants of the search methods particularly well suited to those cases.

5.2.2 Scaling

Fig. 5 shows the performance for two problem sizes. An important question is how rapidly the search cost grows with increasing problem size. An appropriate choice of the scaling is necessary for a study of average behavior so as to include a significant number of hard instances. In this respect, a useful scaling regime is when the number of nogoods specified by the constraints grows linearly with the size of the problem $n$. This corresponds to graph coloring where the number of edges is proportional to the number of nodes, and satisfiability where the number of clauses in the propositional formula is proportional to the number of variables, which have a high concentration of hard search cases [6, 23].

The scaling of the search cost $C$ is shown in Fig. 6. Although the problem sizes feasible for classical simulation may be too small to see the asymptotic growth rate clearly, the search cost appears to grow slowly but still exponentially, on average, for $\alpha = 1$ and 2. Thus, the expected cost grows by about a factor of 10 while the full search space grows in size by a factor of $2^{14}$ over the range of the figure. These values of $\alpha$ correspond to locations just below and just above the peak in the search cost show in Fig. 5.
Figure 6: Log plot of search cost $C$ vs. $n$. The solid curves are for $\alpha = 1$ (gray) and $\alpha = 2$ (black). Each point is the average of 1000 CSPs, except for $n = 22$ with 100 and $n = 24$ with 50. The points include error bars indicating the standard error of estimates of the mean, which in most cases are smaller than the size of the plotted points. The dashed curves are for the CSPs with $m = 0$ (gray) and with $m = m_{\text{max}}$ of Eq. (15) (black).

The dashed curves in Fig. 6 show the behavior for simpler CSPs. In particular, the CSP with the fewest nogoods, i.e., $m = 0$, has a cost just slightly higher than the minimum nogoods problem discussed in the previous section. Although $m = 0$, the CSP still has the necessary nogoods and so has more nogoods in the lattice than the minimum nogoods problem. At the other extreme is the soluble CSP with $m = m_{\text{max}}$ of Eq. (15). Its search cost is about three times larger than that of the maximum nogoods problem of the previous section but shows the same slow growth in search cost. This CSP differs from the maximum nogoods problem only in having no nogoods of size 1, e.g., the sets $\{i\}$ for $i = L+1, \ldots, n$ are nogoods for the maximum nogoods problem but not for the CSP with $m = m_{\text{max}}$ when the prespecified solution is $\{1, \ldots, L\}$.

Overall, we conclude that this algorithm is very effective in concentrating amplitude toward solutions, but it is unclear whether that is enough to give polynomial rather than exponential decrease of $P_{\text{soln}}$, on average, for the hard problems near the transition.

5.2.3 Comparison with Previous Algorithms

Having introduced a new quantum algorithm, an important question is how it compares with previous methods and, in particular, the types of problems for which it is most appropriate. To address this question, Fig. 7 shows how the search cost of this algorithm compares with the scaling of the previous unstructured and structured search methods.

Specifically, to compare with the unstructured method, the number of solutions $S$ was found for each problem instance examined in Fig. 6. The first plot of Fig. 7 shows the ratio $C/\sqrt{N_L}/S$ averaged over the problem instances, where $N_L$ is the number of sets of size $L$. The value $\sqrt{N_L}/S$ characterizes the scaling behavior of the unstructured search among sets at the solution level of the lattice, although
the actual search cost may differ from this by a constant factor \( \delta \). This ratio generally decreases with \( n \), especially for highly constrained problems. If this trend continues for larger \( n \), it would mean the structured algorithm is able to improve search performance by utilizing the problem structure, but definite conclusions cannot be made from these small problem sizes.

The second plot of Fig. 7 compares the new algorithm to the previous structured search algorithm. This previous algorithm is similar in form to the new one, but uses a matrix \( U \) that maps entirely from one level of the lattice to the next at each step, and whose elements have no simple closed form expression. Thus it requires \( J = L \) steps to have any amplitude in solution sets. For comparison, this algorithm was run on the same problems as used in Fig. 6 and the expected search cost \( L/P_{\text{soln}} \) was determined for each problem. The plot shows the ratio of the average search costs of the new and old algorithms. We see that the new algorithm has slightly higher cost, with the relative difference decreasing with \( n \). The difference between the two methods increases as problems become more constrained, but this can be partly offset for highly constrained problems by changing the phase adjustment of Eq. (2) to just invert nogoods. As a further observation from the data used to generate the plot, the two algorithms have comparable variance in search cost within these problem ensembles. At any rate, for a small decrease in performance, the new algorithm provides an analytically simpler search method with the same qualitative behaviors as the previous structured one. This analytic simplicity may facilitate a theoretical analysis of the new algorithm.

### 6 Discussion

The algorithm presented here shows how the underlying lattice structure of search problems can be used as the basis of a structured quantum search algorithm. The algorithm is particularly effective for relatively highly constrained problems. There remain a number of ways in which the algorithm might be improved. First, the initial motivation for the matrix \( U \) was to maximally connect sets to their immediate supersets. In fact, we found that the mapping allowed the algorithm to work best with fewer steps than would be expected from moving up one level at a time in the lattice. It may be possible to design other mappings that do this even more effectively by somewhat reducing the mapping to immediate supersets and increasing the connections to larger supersets.
Another issue is the structure of the types of mappings possible by adjusting the phases of the diagonal matrix $D$. As we saw, this gives matrix elements that depend only on the combination $|r| + |s| − 2|r \cap s|$ when the diagonal elements of $D$ depend only on the size of the corresponding sets. Thus, for instance, there is no way to distinguish mapping from a set to an immediate subset, i.e., moving away from the solution level, from mapping to an immediate superset. For CSPs, another limitation of this mapping is its inability to distinguish necessary nogoods from other sets. Because these nogoods do not depend on particular problem instances, it may be useful to have the matrix $U$ emphasize moving amplitude not just to all immediate supersets equally but rather to focus on those sets that are assignments. Such a modification is likely to be most beneficial for problems with relatively few constraints where the necessary nogoods are a high proportion of all the nogoods in the problem. Thus considering a wider possible range of mappings may allow a more focused search.

There are also a variety of phase adjustment policies. The one studied here is quite effective, but other choices can enhance the performance of the mapping. Furthermore, since we focus on typical or average behavior, other choices that do not improve the average but result in smaller variance would also be useful in improving the predictability of the algorithm’s performance.

As a possible extension to this algorithm, it would be interesting to see whether the nonsolution sets with relatively high probability could be useful also, e.g., as starting points for a local repair type of search [28]. If so, the benefits of this algorithm would be greater than indicated by its direct ability to produce solution sets. This may also suggest similar algorithms for the related optimization problems where the task is to find the best solution according to some metric, not just one consistent with the problem constraints.

Beyond the specific algorithm presented in this paper, the lattice structure provides a general framework for applying quantum computers to search problems. This is due to the many opportunities for using interference among the paths through the lattice to each set at the solution level. Specifically, this search framework could be used to incorporate additional knowledge about the particular problem structure or other search heuristics. This is readily included as a modification to the choice of phases which can be made independently for each state. For example, the choice of phase adjustment policy could be based on the number of constraints in a given problem, i.e., using Eq. (3), unless the problem is highly constrained. In this latter case, we could just invert nogoods only, resulting in somewhat better performance.

Changes to the mapping that mixes amplitude among sets are more complicated due to the requirement to maintain unitarity (as well as computational simplicity). Nevertheless, when a heuristic works well classically for a particular class of problems, it suggests a corresponding unitary mapping that is as close as possible to the classical procedure the heuristic uses to move from one state to the next during search. This method for constructing quantum search mappings was the underlying motivation for the specific map used in the structured search presented here. For example, it would be interesting to examine maps motivated by classical repair and abstraction search methods.

Another way to incorporate heuristics is by changing the initial condition. In the method reported here, initially all amplitude is in the empty set. Other possibilities include starting with amplitude in the consistent sets at the level of the lattice corresponding to the nogoods directly determined by the constraints [21] or starting with an equal superposition in all sets of the lattice [17].

There remain a number of important questions. First, how are the results degraded by errors and decoherence, the major difficulties for the construction of quantum computers [24, 33, 15, 50]? While there has been recent progress in implementation [1, 8, 9, 16, 34], quantum approaches to error control [1, 22] and studies of decoherence in the context of factoring [4], it remains to be seen how these problems affect the framework presented here.

Second, it would be useful to have a theory for asymptotic behavior of this algorithm for large $n$, even
if only approximately in the spirit of mean-field theories of physics. This would give a better indication of the scaling behavior than the classical simulations, necessarily limited to small cases, and may also suggest better phase choices. Considering these questions may suggest simple modifications to the quantum map to improve its robustness and scaling. There thus remain many options to explore for using the deep structure of combinatorial search problems as the basis for general quantum search methods.

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