Quantum walk speedup of backtracking algorithms

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Constraint satisfaction problems

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- We might want to find one assignment to the variables that satisfies all the constraints, or list all such assignments.

- For many CSPs, the best algorithms known for either task have exponential runtime in \( n \).

- A fundamental example: boolean satisfiability with at most 3 variables per clause (3-SAT).

\[
(x_1 \lor x_2) \land (x_1 \lor \neg x_3) \land (\neg x_1 \lor \neg x_2 \lor x_4) \land (x_2 \lor x_3)
\]
A naïve algorithm

$$(x_1 \lor x_2) \land (x_1 \lor \neg x_3) \land (\neg x_1 \lor \neg x_2 \lor x_4) \land (x_2 \lor x_3)$$

Imagine we want to find all satisfying assignments. One naïve way of doing this is exhaustive search:
A less naïve algorithm

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Some paths in this tree are disallowed early on...

- For example, if we set \(x_1 = 0, x_2 = 0\), we already know the formula is false.
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- For example, if we set \(x_1 = 0, x_2 = 0\), we already know the formula is **false**.

- We can modify the above algorithm to explore a smaller tree by checking whether the formula is true (or false) at **internal nodes** in the tree.
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- Exploring the tree corresponds to substituting variable values into the formula.

- At each vertex, we determine which variable to choose next using a heuristic.
A less naïve algorithm

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Imagine we use the following heuristic: choose an arbitrary variable in a shortest clause.
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This algorithm is a simple variant of the DPLL algorithm, which forms the basis of many of the most efficient SAT solvers used in practice.
```
General backtracking framework

Suppose we want to solve a constraint satisfaction problem on $n$ variables, each picked from $[d] := \{0, \ldots, d - 1\}$.

- Write $\mathcal{D} := ([d] \cup \{\ast\})^n$, where $\ast$ means “not assigned yet”.

Assume we have access to a predicate $P : \mathcal{D} \rightarrow \{\text{true}, \text{false}, \text{indeterminate}\}$ which tells us the status of a partial assignment. Also assume we have access to a heuristic $h : \mathcal{D} \rightarrow \{1, \ldots, n\}$ which returns the next index to branch on from a given partial assignment. Also allows randomised heuristics, as distributions over deterministic functions $h$. 
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Main result

Theorem

Let $T$ be the number of vertices in the backtracking tree. Then there is a bounded-error quantum algorithm which evaluates $P$ and $h O(\sqrt{T}n^{3/2} \log n)$ times each, and outputs $x$ such that $P(x)$ is true, or “not found” if no such $x$ exists.

If we are promised that there exists a unique $x_0$ such that $P(x_0)$ is true, this is improved to $O(\sqrt{T}n \log n)$. In both cases the algorithm uses $\text{poly}(n)$ space and $\text{poly}(n)$ auxiliary quantum gates per use of $P$ and $h$.

The algorithm can be modified to find all solutions by striking out previously seen solutions. We usually think of $T$ as being exponentially large in $n$. In this regime, this is a near-quadratic separation.

Note that the algorithm does not need to know $T$. 


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- Note that the algorithm does not need to know $T$. 
Some previous works have developed quantum algorithms related to backtracking:

- [Cerf, Grover and Williams ’00] developed a quantum algorithm for constraint satisfaction problems, based on a nested version of Grover search. This can be seen as a quantum version of one particular backtracking algorithm that runs quadratically faster.
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By contrast, the algorithm presented here achieves a (nearly) *quadratic* separation for all trees.
Search in the backtracking tree

Idea: Use quantum search to find a marked vertex (i.e. solution) in the tree produced by the backtracking algorithm.
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These can be overcome using work of [Belovs ’13] relating quantum walks to effective resistance in an electrical network.
Quantum walk in a tree

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- $D_r = I - 2|\psi_r\rangle\langle\psi_r|$, where

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Let $A$ and $B$ be the sets of vertices an even and odd distance from the root, respectively.

Then a step of the walk consists of applying the operator $R_B R_A$, where $R_A = \bigoplus_{x \in A} D_x$ and $R_B = |r\rangle \langle r| + \bigoplus_{x \in B} D_x$. 
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Using the walk

We apply phase estimation to $R_B R_A$ on state $|r\rangle$ with precision $O(1/\sqrt{Tn})$, where $n$ is an upper bound on the depth of the tree, and accept if the eigenvalue is 1.
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**Claim (special case of [Belovs ’13])**

- If there is a marked vertex, $R_B R_A$ has a normalised eigenvector with eigenvalue 1 and overlap $\geq \frac{1}{2}$ with $|r\rangle$. 

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- If there is no marked vertex, $\|P_\chi |r\rangle\|^2 \leq \frac{1}{4}$, where $P_\chi$ is the projector onto the space spanned by eigenvectors of $R_B R_A$ with eigenvalue $e^{2i\theta}$, for $|\theta| \leq 1/(2\sqrt{Tn})$. 
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We apply phase estimation to $R_BR_A$ on state $|r\rangle$ with precision $O(1/\sqrt{Tn})$, where $n$ is an upper bound on the depth of the tree, and accept if the eigenvalue is 1.

Claim (special case of [Belovs '13])

- If there is a marked vertex, $R_BR_A$ has a normalised eigenvector with eigenvalue 1 and overlap $\geq \frac{1}{2}$ with $|r\rangle$.

- If there is no marked vertex, $\|P_X|r\rangle\|^2 \leq \frac{1}{4}$, where $P_X$ is the projector onto the space spanned by eigenvectors of $R_BR_A$ with eigenvalue $e^{2i\theta}$, for $|\theta| \leq 1/(2\sqrt{Tn})$.

It follows that we can use the above subroutine to detect a marked vertex with $O(\sqrt{Tn})$ uses of $R_BR_A$. 
From detection to search

- We can use the above detection procedure as a subroutine to find marked vertices in the tree, via binary search.
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- We can use the above detection procedure as a subroutine to find marked vertices in the tree, via binary search.

- We first apply the procedure to the whole tree. If it outputs “marked vertex exists” we apply it to the subtree rooted at each of the children of the root in turn and repeat.

- There is a more efficient algorithm if there is exactly one marked vertex, using the fact that the eigenvector with eigenvalue 1 encodes the entire path from the root to the marked vertex.
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We can now use this search algorithm to speed up the classical backtracking algorithm:

- Recall that we have access to $P$ and $h$.

- Represent each vertex in the tree by a string $(i_1, v_1), \ldots, (i_\ell, v_\ell)$ giving the indices and values of the variables set so far.

- Then we can use $P$ and $h$ to determine the neighbours of each vertex. This allows us to implement the $D_x$ operations (efficiently).
Summary and open problems

- If we have a classical backtracking algorithm whose tree has $T$ vertices, there is a quantum algorithm which finds a solution in time $O(\sqrt{T \text{poly}(n)})$.

Open problems:

- What if the classical algorithm is lucky and finds a solution early on?
- Can we improve the runtime for finding a solution to the best possible $O(\sqrt{Tn})$?
- If there are $k$ solutions, can we find them all in time $O(\sqrt{Tnk})$?
- What else can we do using the electrical circuit framework of [Belovs '13]?
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- If we have a classical backtracking algorithm whose tree has $T$ vertices, there is a quantum algorithm which finds a solution in time $O(\sqrt{T} \text{poly}(n))$.

- This algorithm speeds up DPLL, the basis of many of the fastest SAT solvers used in practice.

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- What else can we do using the electrical circuit framework of [Belovs ‘13]?
Thanks!

Pic: Wikipedia
General backtracking framework

**Backtracking algorithm**

Return $\text{bt}(\ast^n)$, where $\text{bt}$ is the following recursive procedure:

$\text{bt}(x)$:

1. If $P(x)$ is true, output $x$ and return.
2. If $P(x)$ is false, return.
3. Set $j = h(x)$.
4. For each $w \in [d]$:
   1. Set $y$ to $x$ with the $j$'th entry replaced with $w$.
   2. Call $\text{bt}(y)$.

This algorithm runs in time at most $O(d^n)$, but on some instances its runtime can be substantially lower.
Exponentially reduced average runtime

The above algorithm has an \textit{instance-dependent} runtime: If the classical algorithm uses time $T$ on a given problem instance, the quantum algorithm uses time $O(\sqrt{T} \text{poly}(n))$. This can be leveraged to obtain exponential reductions in expected runtime. We consider a setting where the input is picked from some distribution, and we are interested in the average runtime of the algorithm, over the input distribution. Claim: Pick a random 3-SAT instance on $n$ variables by choosing $m = m'$ random clauses, where $\Pr[m = m'] \propto 2^{-Cn^3/2/\sqrt{m'}}$. Then there exists a constant $C$ such that the expected quantum runtime is $\text{poly}(n)$, but a simple backtracking algorithm has expected runtime exponential in $n$. 
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Claim

Pick a random 3-SAT instance on $n$ variables by choosing $m$ random clauses, where $\Pr[m = m'] \propto 2^{-C n^{3/2}/\sqrt{m'}}$.

Then there exists a constant $C$ such that the expected quantum runtime is $\text{poly}(n)$, but a simple backtracking algorithm has expected runtime exponential in $n$. 
From quadratic to exponential speedups?

For example:

- Let $T(X)$ denote the number of vertices in the backtracking tree on input $X$. 

$\text{So for } \beta > -2 \text{ the average classical complexity is large.}$

$\text{But, if } -2 < \beta < -3/2, \text{ the average number of steps used }$

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$\mathbb{E}_X[T(X)] \leq \sum_{t \geq 1} O(\sqrt{t} \cdot t^{\beta} \text{poly}(n)) = \text{poly}(n)$.
From quadratic to exponential speedups?

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Proof: marked element case

Claim

Let $x_0$ be a marked element. Then

$$|\phi\rangle = \sqrt{n}|r\rangle + \sum_{x \neq r, x \sim x_0} (-1)^{\ell(x)}|x\rangle$$

is an eigenvector of $R_B R_A$ with eigenvalue 1, where $\ell(x)$ is the distance of $x$ from the root.
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- Also,
  \[
  \frac{\langle r | \phi \rangle}{\| |\phi\rangle\|} \geq \frac{1}{\sqrt{2}}.
  \]
Proof: no marked element case

**Effective spectral gap lemma** [Lee et al. ’11]

Set $R_A = 2\Pi_A - I$, $R_B = 2\Pi_B - I$. Let $P_\chi$ be the projector onto the span of the eigenvectors of $R_B R_A$ with eigenvalues $e^{2i\theta}$ such that $|\theta| \leq \chi$. Then, for any $|\psi\rangle$ such that $\Pi_A |\psi\rangle = 0$, we have

$$\|P_\chi \Pi_B |\psi\rangle\| \leq \chi \| |\psi\rangle\|.$$
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- Here $|\psi_x^\perp\rangle$ is orthogonal to $|\psi_x\rangle$ and has support only on $\{ |x\rangle \} \cup \{ |y\rangle : x \rightarrow y \}$; in addition to $|r\rangle$ in the case of $R_B$. 
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- By the effective spectral gap lemma,

$$\|P_\chi |r\rangle\| = \|P_\chi \Pi_B |\eta\rangle\| \leq \chi |||\eta\rangle|| \leq \chi \sqrt{Tn}.$$