Exact results for accepting probabilities of quantum automata

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Abstract

One of the properties of the Kondacs-Watrous model of quantum finite automata (QFA) is that the probability of the correct answer for a QFA cannot be amplified arbitrarily. In this paper, we determine the maximum probabilities achieved by QFAs for several languages. In particular, we show that any language that is not recognized by an RFA (reversible finite automaton) can be recognized by a QFA with probability at most 0.7726....

Key words: quantum computation, finite automata, quantum measurement.

1 Introduction

A quantum finite automaton (QFA) is a model for a quantum computer with a finite memory. QFAs can recognize the same languages as classical finite automata but they can be exponentially more space efficient than their classical counterparts [AF 98].
To recognize an arbitrary regular language, QFAs need to be able to perform general measurements after reading every input symbol, as in [AW 01, C 01, P 99]. If we restrict QFAs to unitary evolution and one measurement at the end of computation (which might be easier to implement experimentally), their power decreases considerably. Namely [CM 97, BP 99], they can only recognize the languages recognized by permutation automata, a classical model in which the transitions between the states have to be fully reversible.

Similar decreases of the computational power have been observed in several other contexts. Quantum error correction is possible if we have a supply of quantum bits initialized to $|0\rangle$ at any moment of computation (see chapter 10 of [NC 00]). Yet, if the number of quantum bits is fixed and it is not allowed to re-initialize them by measurements, error correction becomes difficult [ABIN 96]. Simulating a probabilistic Turing machine by a quantum Turing machine is trivial if we allow to measure and reinitialize qubits but quite difficult if the number of qubits is fixed and they cannot be reinitialized [W 98].

Thus, the availability of measurements is very important for quantum automata. What happens if the measurements are allowed but restricted? How can we use the measurements of a restricted form to enhance the abilities of quantum automata? Can quantum effects be used to recognize languages that are not recognizable by classical automata with the same reversibility requirements?

In this paper, we look at those questions for “measure-many” QFA model by Kondacs and Watrous [KW 97]. This model allows intermediate measurements during the computation but these measurements have to be of a restricted type. More specifically, they can have 3 outcomes: “accept”, “reject”, “don’t halt” and if one gets “accept” or “reject”, the computation ends and this is the result of computation. The reason for allowing measurements of this type was that the states of a QFA then have a simple description of the form $(|\psi\rangle, p_a, p_r)$ where $p_a$ is the probability that the QFA has accepted, $p_r$ is the probability that the QFA has rejected and $|\psi\rangle$ is the remaining state if the automaton has not accepted or rejected. Allowing more general measurements would make the remaining state a mixed state $\rho$ instead of a pure state $|\psi\rangle$. Having a mixed state as the current state of a QFA is very reasonable physically but the mathematical apparatus for handling pure states is simpler than one for mixed states.

For this model, it is known that [AF 98]

- Any language recognizable by a QFA with a probability $7/9 + \epsilon$, $\epsilon > 0$ is recognizable by a reversible finite automaton (RFA).

For the rest of this paper, we will refer to “measure-many” QFAs as simply QFAs because this is the only model considered in this paper.
• The language $a^*b^*$ can be recognized with probability 0.6822... but cannot be recognized by an RFA.

Thus, the quantum automata in this model have an advantage over their classical counterparts (RFAs) with the same reversibility requirements but this advantage only allows to recognize languages with probabilities at most $7/9$, not $1 - \epsilon$ with arbitrary $\epsilon > 0$. This is a quite unusual property because, in almost any other computational model, the accepting probability can be increased by repeating the computation in parallel. As we see, this is not the case for QFAs.

In this paper, we develop a method for determining the maximum probability with which a QFA can recognize a given language. Our method is based on the quantum counterpart of classification of states of a Markov chain into ergodic and transient states [KS 76]. We use this classification of states to transform the problem of determining the maximum accepting probability of a QFA into a quadratic optimization problem. Then, we solve this problem (analytically in simpler cases, by computer in more difficult cases).

Compared to previous work, our new method has two advantages. First, it gives a systematic way of calculating the maximum accepting probabilities. Second, solving the optimization problems usually gives the maximum probability exactly. Most of previous work [AF 98,ABFK 99] used approaches depending on the language and required two different methods: one for bounding the probability from below, another for bounding it from above. Often, using two different approaches gave an upper and a lower bound with a gap between them (like 0.6822... vs. $7/9 + \epsilon$ mentioned above). With the new approach, we are able to close those gaps.

We use our method to calculate the maximum accepting probabilities for a variety of languages (and classes of languages).

First, we construct a quadratic optimization problem for the maximum accepting probability by a QFA of a language that is not recognizable by an RFA. Solving the problem gives the probability $(52 + 4\sqrt{7})/81 = 0.7726...$. This probability can be achieved for the language $a^+$ in the two-letter alphabet $\{a,b\}$ but no language that is not recognizable by a RFA can be recognized with a higher probability. This improves the $7/9 + \epsilon$ result of [AF 98].

This result can be phrased in a more general way. Namely, we can find the property of a language which makes it impossible to recognize the language by an RFA. This property can be nicely stated in the form of the minimal deterministic automaton containing a fragment of a certain form.

We call such a fragment a “non-reversible construction”. It turns out that there are many different “non-reversible constructions” and they have dif-
ferent influence on the accepting probability. The one contained in the \( a^+ \) language makes the language not recognizable by an RFA but the language is still recognizable by a QFA with probability 0.7726... In contrast, some constructions analyzed in [BP 99,AKV 01] make the language not recognizable with probability \( 1/2 + \epsilon \) for any \( \epsilon > 0 \).

In the rest of this paper, we look at different “non-reversible constructions” and their effects on the accepting probabilities of QFAs. We consider three constructions: “two cycles in a row”, “\( k \) cycles in parallel” and a variant of the \( a^+ \) construction. The best probabilities with which one can recognize languages containing these constructions are 0.6894..., \( k/(2k - 1) \) and 0.7324..., respectively.

The solution of the optimization problem for “two cycles in a row” gives a new QFA for the language \( a^*b^* \) that recognizes it with probability 0.6894..., improving the result of [AF 98]. Again, using the solution of the optimization problem gives a better QFA that was previously missed because of disregarding some parameters.

## 2 Preliminaries

### 2.1 Quantum automata

We define the Kondacs-Watrous (“measure-many”) model of QFAs [KW 97].

A QFA is a tuple \( M = (Q; \Sigma; V; q_0; Q_{\text{acc}}; Q_{\text{rej}}) \) where \( Q \) is a finite set of states, \( \Sigma \) is an input alphabet, \( V \) is a transition function (explained below), \( q_0 \in Q \) is a starting state, and \( Q_{\text{acc}} \subseteq Q \) and \( Q_{\text{rej}} \subseteq Q \) are sets of accepting and rejecting states (\( Q_{\text{acc}} \cap Q_{\text{rej}} = \emptyset \)). The states in \( Q_{\text{acc}} \) and \( Q_{\text{rej}} \) are called halting states and the states in \( Q_{\text{non}} = Q - (Q_{\text{acc}} \cup Q_{\text{rej}}) \) are called non halting states.

**States of \( M \).** The state of \( M \) can be any superposition of states in \( Q \) (i.e., any linear combination of them with complex coefficients). We use \( |q\rangle \) to denote the superposition consisting of state \( q \) only. \( l_2(Q) \) denotes the linear space consisting of all superpositions, with \( l_2 \)-distance on this linear space.

**Endmarkers.** Let \( \kappa \) and \$ be symbols that do not belong to \( \Sigma \). We use \( \kappa \) and \$ as the left and the right endmarker, respectively. We call \( \Gamma = \Sigma \cup \{\kappa; \$\} \) the working alphabet of \( M \).

**Transition function.** The transition function \( V \) is a mapping from \( \Gamma \times l_2(Q) \) to \( l_2(Q) \) such that, for every \( a \in \Gamma \), the function \( V_a : l_2(Q) \to l_2(Q) \) defined by
\( V_a(x) = V(a, x) \) is a unitary transformation (a linear transformation on \( l_2(Q) \) that preserves \( l_2 \) norm).

**Computation.** The computation of a QFA starts in the superposition \( |q_0\rangle \). Then transformations corresponding to the left endmarker \( \kappa \), the letters of the input word \( x \) and the right endmarker \( \$ \) are applied. The transformation corresponding to \( a \in \Gamma \) consists of two steps.

1. First, \( V_a \) is applied. The new superposition \( \psi' \) is \( V_a(\psi) \) where \( \psi \) is the superposition before this step.

2. Then, \( \psi' \) is observed with respect to \( E_{\text{acc}}, E_{\text{rej}}, E_{\text{non}} \) where \( E_{\text{acc}} = \text{span}\{ |q\rangle : q \in Q_{\text{acc}} \}, E_{\text{rej}} = \text{span}\{ |q\rangle : q \in Q_{\text{rej}} \}, E_{\text{non}} = \text{span}\{ |q\rangle : q \in Q_{\text{non}} \} \). It means that if the system’s state before the measurement was

\[
\psi' = \sum_{q_i \in Q_{\text{acc}}} \alpha_i |q_i\rangle + \sum_{q_j \in Q_{\text{rej}}} \beta_j |q_j\rangle + \sum_{q_k \in Q_{\text{non}}} \gamma_k |q_k\rangle
\]

then the measurement accepts \( \psi' \) with probability \( p_a = \Sigma \alpha_i^2 \), rejects with probability \( p_r = \Sigma \beta_j^2 \) and continues the computation (applies transformations corresponding to next letters) with probability \( p_c = \Sigma \gamma_k^2 \) with the system having the (normalized) state \( \frac{\psi}{\| \psi \|} \) where \( \psi = \Sigma \gamma_k |q_k\rangle \).

We regard these two transformations as reading a letter \( a \).

**Notation.** We use \( V'_a \) to denote the transformation consisting of \( V_a \) followed by projection to \( E_{\text{non}} \). This is the transformation mapping \( \psi \) to the non-halting part of \( V_a(\psi) \). We use \( V'_w \) to denote the product of transformations \( V'_w = V'_a_n V'_a_{n-1} \ldots V'_a_2 V'_a_1 \), where \( a_i \) is the \( i \)-th letter of the word \( w \).

We also use \( \psi_w \) to denote the (unnormalized) non-halting part of QFA’s state after reading the left endmarker \( \kappa \) and the word \( w \in \Sigma^* \). From the notation it follows that \( \psi_w = V'_{\kappa w} (|q_0\rangle) \).

**Recognition of languages.** We will say that an automaton recognizes a language \( L \) with probability \( p \) \((p > \frac{1}{2})\) if it accepts any word \( x \in L \) with probability \( \geq p \) and rejects any word \( x \notin L \) with probability \( \geq p \).

2.2 Useful lemmas

For classical Markov chains, one can classify the states of a Markov chain into **ergodic** sets and **transient** sets [KS 76]. If the Markov chain is in an ergodic set, it never leaves it. If it is in a transient set, it leaves it with probability \( 1 - \epsilon \) for an arbitrary \( \epsilon > 0 \) after sufficiently many steps.
A quantum counterpart of a Markov chain is a quantum system to which we repeatedly apply a transformation that depends on the current state of the system but does not depend on previous states. In particular, it can be a QFA that repeatedly reads the same word $x$. Then, the state after reading $x \cdot k + 1$ times depends on the state after reading $x \cdot k$ times but not on any of the states before that. The next lemma gives the classification of states for such QFAs.

**Lemma 1** [AF 98] Let $x \in \Sigma^+$. There are subspaces $E_1, E_2$ such that $E_{\text{non}} = E_1 \oplus E_2$ and

(i) If $\psi \in E_1$, then $V_x'(\psi) \in E_1$ and $\|V_x'(\psi)\| = \|\psi\|$,  
(ii) If $\psi \in E_2$, then $\|V_x^k(\psi)\| \to 0$ when $k \to \infty$.

Instead of ergodic and transient sets, we have subspaces $E_1$ and $E_2$. The subspace $E_1$ is a counterpart of an ergodic set: if the quantum process defined by repeated reading of $x$ is in a state $\psi \in E_1$, it stays in $E_1$. $E_2$ is a counterpart of a transient set: if the state is $\psi \in E_2$, $E_2$ is left (for an accepting or rejecting state) with probability arbitrarily close to 1 after sufficiently many $x$’s.

In some of proofs we also use a generalization of Lemma 1 to the case of two (or more) words $x$ and $y$:

**Lemma 2** [AKV 01] Let $x, y \in \Sigma^+$. There are subspaces $E_1, E_2$ such that $E_{\text{non}} = E_1 \oplus E_2$ and

(i) If $\psi \in E_1$, then $V_x'(\psi) \in E_1$ and $V_y'(\psi) \in E_1$ and $\|V_x'(\psi)\| = \|\psi\|$ and $\|V_y'(\psi)\| = \|\psi\|$,  
(ii) If $\psi \in E_2$, then for any $\epsilon > 0$, there exists $t \in (x|y)^*$ such that $\|V_t'(\psi)\| < \frac{\epsilon}{e}$.

We also use a lemma from [BV 97].

**Lemma 3** [BV 97] If $\psi$ and $\phi$ are two quantum states and $\|\psi - \phi\| < \epsilon$ then the total variational distance between probability distributions generated by the same measurement on $\psi$ and $\phi$ is at most $\frac{4}{\epsilon}$.

### 3 QFAs vs. RFAs

Ambainis and Freivalds [AF 98] characterized the languages recognized by RFAs as follows.

\footnote{The lemma in [BV 97] has $4\varepsilon$ but it can be improved to $2\varepsilon$.}
**Theorem 4** [AF 98] Let \( L \) be a language and \( M \) be its minimal automaton. \( L \) is recognizable by a RFA if and only if there is no \( q_1, q_2, x \) such that

1. \( q_1 \neq q_2 \),
2. If \( M \) starts in the state \( q_1 \) and reads \( x \), it passes to \( q_2 \),
3. If \( M \) starts in the state \( q_2 \) and reads \( x \), it passes to \( q_2 \), and
4. \( q_2 \) is neither ”all-accepting” state, nor ”all-rejecting” state,

An RFA is a special case of a QFA that outputs the correct answer with probability 1. Thus, any language that does not contain the construction of Theorem 4 can be recognized by a QFA that always outputs the correct answer. Ambainis and Freivalds [AF 98] also showed the reverse of this: any language \( L \) with the minimal automaton containing the construction of Theorem 4 cannot be recognized by a QFA with probability \( 7/9 + \epsilon \).

We consider the question: what is the maximum probability of correct answer than can be achieved by a QFA for a language that cannot be recognized by an RFA? The answer is:

**Theorem 5** Let \( L \) be a language and \( M \) be its minimal automaton.

1. If \( M \) contains the construction of Theorem 4, \( L \) cannot be recognized by a 1-way QFA with probability more than \( p = (52 + 4\sqrt{7})/81 = 0.7726... \)
2. There is a language \( L \) with the minimal automaton \( M \) containing the construction of Theorem 4 that can be recognized by a QFA with probability \( p = (52 + 4\sqrt{7})/81 = 0.7726... \)

**Proof.** We consider the following optimization problem.

**Optimization problem 1.** Find the maximum \( p \) such that there is a finite dimensional vector space \( E_{opt} \), subspaces \( E_a, E_r \) such that \( E_a \perp E_r \), vectors \( v_1, v_2 \) such that \( v_1 \perp v_2 \) and \( \|v_1 + v_2\| = 1 \) and probabilities \( p_1, p_2 \) such that \( p_1 + p_2 = \|v_2\|^2 \) and

1. \( \|P_a(v_1 + v_2)\|^2 \geq p \),
2. \( \|P_r(v_1)\|^2 + p_2 \geq p \),
3. \( p_2 \leq 1 - p \).

We sketch the relation between a QFA recognizing \( L \) and this optimization problem. Let \( Q \) be a QFA recognizing \( L \). Let \( p_{min} \) be the minimum probability of the correct answer for \( Q \), over all words. We use \( Q \) to construct an instance of the optimization problem above with \( p \geq p_{min} \).
Namely, we look at $Q$ reading an infinite (or very long finite) sequence of letters $x$. By Lemma 1, we can decompose the starting state $\psi$ into 2 parts $\psi_1 \in E_1$ and $\psi_2 \in E_2$. Define $v_1 = \psi_1$ and $v_2 = \psi_2$. Let $p_1$ and $p_2$ be the probabilities of getting into an accepting (for $p_1$) or rejecting (for $p_2$) state while reading an infinite sequence of $x$’s starting from the state $v_2$. The second part of Lemma 1 implies that $p_1 + p_2 = \|v_2\|^2$.

Since $q_1$ and $q_2$ are different states of the minimal automaton $M$, there is a word $y$ that is accepted in one of them but not in the other. Without loss of generality, we assume that $y$ is accepted if $M$ is started in $q_1$ but not if $M$ is started in $q_2$. Also, since $q_2$ is not an “all-accepting” state, there must be a word $z$ that is rejected if $M$ is started in the state $q_2$.

We choose $E_a$ and $E_r$ so that the square of the projection $P_a (P_r)$ of a vector $v$ on $E_a (E_r)$ is equal to the accepting (rejecting) probability of $Q$ if we run $Q$ on the starting state $v$ and input $y$ and the right endmarker $\$. 

Finally, we set $p$ equal to the inf of the set consisting of the probabilities of correct answer of $Q$ on the words $y$ and $x^iy, x^iz$ for all $i \in \mathbb{Z}$.

Then, Condition 1 of the optimization problem, $\|P_a(v_1 + v_2)\|^2 \geq p$ is true because the word $y$ must be accepted and the accepting probability for it is exactly the square of the projection of the starting state $(v_1 + v_2)$ to $P_a$.

Condition 2 follows from running $Q$ on a word $x^iy$ for some large $i$. By Lemma 1, if $i > k$ for some $k$, $\|V'_{x^i}(v_2)\| \leq \epsilon$. Also, $v_1, V'_{x^i}(v_1), V'_{x^2}(v_1), \ldots$ is an infinite sequence in a finite-dimensional space. Therefore, it has a limit point and there are $i, j, i \geq k$ such that 

$$\|V'_{x^i}(v_1) - V'_{x^{i+j}}(v_1)\| \leq \epsilon.$$ 

We have 

$$V'_{x^j}(v_1) - V'_{x^{i+j}}(v_1) = V'_{x^j}(v_1 - V'_{x^i}(v_1)).$$

Since $\|V'_{x^i}(\psi)\| = \|\psi\|$ for $\psi \in E_1$, $\|V'_{x^i}(v_1 - V'_{x^i}(v_1))\| = \|v_1 - V'_{x^i}(v_1)\|$ and we have 

$$\|v_1 - V'_{x^i}(v_1)\| \leq \epsilon.$$ 

Thus, reading $x^i$ has the following effect:

1. $v_1$ gets mapped to a state that is at most $\epsilon$-away (in $l_2$ norm) from $v_1$,
2. $v_2$ gets mapped to an accepting/rejecting state and most $\epsilon$ fraction of it stays on the non-halting states.
Together, these two requirements mean that the state of $Q$ after reading $x^i$ is at most $2\epsilon$-away from $v_1$. Also, the probabilities of $Q$ accepting and rejecting while reading $x^i$ differ from $p_1$ and $p_2$ by at most $\epsilon$.

Let $p_{x^iy}$ be the probability of $Q$ rejecting $x^iy$. Since reading $y$ in $q_2$ leads to a rejection, $x^iy$ must be rejected and $p_{x^iy} \geq p$. The probability $p_{x^iy}$ consists of two parts: the probability of rejection during $x^i$ and the probability of rejection during $y$. The first part differs from $p_2$ by at most $\epsilon$, the second part differs from $\|P_r(v_1)\|^2$ by at most $4\epsilon$ (because the state of $Q$ when starting to read $y$ differs from $v_1$ by at most $2\epsilon$ and, by Lemma 3, the accepting probabilities differ by at most twice that). Therefore,

$$p_{x^iy} - 5\epsilon \leq p_2 + \|P_r(v_1)\|^2 \leq p_{x^iy} + 5\epsilon.$$

Since $p_{x^iy} \geq p$, this implies $p - 5\epsilon \leq p_2 + \|P_r(v_1)\|^2$. By appropriately choosing $i$, we can make this true for any $\epsilon > 0$. Therefore, we have $p \leq p_2 + \|P_r(v_1)\|^2$ which is Condition 2.

Condition 3 is true by considering $x^iz$. This word must be accepted with probability $p$. Therefore, for any $i$, $Q$ can only reject during $x^i$ with probability $1 - p$ and $p_2 \leq 1 - p$.

This shows that no QFA can achieve a probability of correct answer more than the solution of optimization problem 1. It remains to solve this problem.

**Solving Optimization problem 1.**

The key idea is to show that it is enough to consider 2-dimensional instances of the problem.

Since $v_1 \perp v_2$, the vectors $v_1, v_2, v_1 + v_2$ form a right-angled triangle. This means that $\|v_1\| = \cos \beta \|v_1 + v_2\| = \cos \beta, \|v_2\| = \sin \beta \|v_1 + v_2\| = \sin \beta$ where $\beta$ is the angle between $v_1$ and $v_1 + v_2$. Let $w_1$ and $w_2$ be the normalized versions of $v_1$ and $v_2$: $w_1 = \frac{v_1}{\|v_1\|}, \ w_2 = \frac{v_2}{\|v_2\|}$. Then, $v_1 = \cos \beta w_1$ and $v_2 = \sin \beta w_2$.

Consider the two-dimensional subspace spanned by $P_a(w_1)$ and $P_r(w_1)$. Since the accepting and the rejecting subspaces $E_a$ and $E_r$ are orthogonal, $P_a(w_1)$ and $P_r(w_1)$ are orthogonal. Therefore, the vectors $w_a = \frac{P_a(w_1)}{\|P_a(w_1)\|}$ and $w_r = \frac{P_r(w_1)}{\|P_r(w_1)\|}$ form an orthonormal basis. We write the vectors $w_1, v_1$ and $v_1 + v_2$ in this basis. The vector $w_1$ is $(\cos \alpha, \sin \alpha)$ where $\alpha$ is the angle between $w_1$ and $w_a$. The vector $v_1 = \cos \beta w_1$ is equal to $(\cos \beta \cos \alpha, \cos \beta \sin \alpha)$.

Next, we look at the vector $v_1 + v_2$. We fix $\alpha, \beta$ and $v_1$ and try to find the $v_2$ which maximizes $p$ for the fixed $\alpha, \beta$ and $v_1$. The only place where $v_2$ appears in the optimization problem 1 is $\|P_a(v_1 + v_2)\|^2$ on the left hand side.
of Condition 1. Therefore, we should find \( v_2 \) that maximizes \( \|P_a(v_1 + v_2)\|^2 \).

We have two cases:

1. \( \alpha \geq \beta \).

   The angle between \( v_1 + v_2 \) and \( w_a \) is at least \( \alpha - \beta \) (because the angle between \( v_1 \) and \( w_a \) is \( \alpha \) and the angle between \( v_1 + v_2 \) and \( v_1 \) is \( \beta \)). Therefore, the projection of \( v_1 + v_2 \) to \( w_a \) is at most \( \cos(\alpha - \beta) \). Since \( w_r \) is a part of the rejecting subspace \( E_r \), this means that \( \|P_a(v_1 + v_2)\|^2 \leq \cos^2(\alpha - \beta) \). The maximum \( \|P_a(v_1 + v_2)\|^2 = \cos^2(\alpha - \beta) \) is achieved if we put \( v_1 + v_2 \) in the plane spanned by \( w_a \) and \( w_r \): \( v_1 + v_2 = (\cos(\alpha - \beta), \sin(\alpha - \beta)) \).

   Next, we can rewrite Condition 3 of the optimization problem as \( 1 - p_2^2 \geq p \). Then, Conditions 1-3 together mean that

   \[
   p = \min(\|P_a(v_1 + v_2)\|^2, \|P_r(v_1)\|^2 + p_2, 1 - p_2). \tag{1}
   \]

   To solve the optimization problem, we have to maximize \( (1) \) subject to the conditions of the problem. From the expressions for \( v_1 \) and \( v_1 + v_2 \) above, it follows that \( (1) \) is equal to

   \[
   p = \min(\cos^2(\alpha - \beta), \sin^2 \alpha \cos^2 \beta + p_2, 1 - p_2) \tag{2}
   \]

   First, we maximize \( \min(\sin^2 \alpha \cos^2 \beta + p_2, 1 - p_2) \). The first term is increasing in \( p_2 \), the second is decreasing. Therefore, the maximum is achieved when both become equal which happens when \( p_2 = \frac{1 - \sin^2 \alpha \cos^2 \beta}{2} \). Then, both \( \sin^2 \alpha \cos^2 \beta + p_2 \) and \( 1 - p_2 \) are \( \frac{1 + \sin^2 \alpha \cos^2 \beta}{2} \). Now, we have to maximize

   \[
   p = \min \left( \cos^2(\alpha - \beta), \frac{1 + \sin^2 \alpha \cos^2 \beta}{2} \right). \tag{3}
   \]

   We first fix \( \alpha - \beta \) and try to optimize the second term. Since \( \sin \alpha \cos \beta = \frac{\sin(\alpha + \beta) + \sin(\alpha - \beta)}{2} \) (a standard trigonometric identity), it is maximized when \( \alpha + \beta = \frac{\pi}{2} \) and \( \sin(\alpha + \beta) = 1 \). Then, \( \beta = \frac{\pi}{2} - \alpha \) and \( (3) \) becomes

   \[
   p = \min \left( \sin^2 2\alpha, \frac{1 + \sin^4 \alpha}{2} \right). \tag{4}
   \]

   The first term is increasing in \( \alpha \), the second is decreasing. The maximum is achieved when

   \[
   \sin^2 2\alpha = \frac{1 + \sin^4 \alpha}{2}. \tag{5}
   \]

   The left hand side of \( (5) \) is equal to \( 4 \sin^2 \alpha \cos^2 \alpha = 4 \sin^2 \alpha (1 - \sin^2 \alpha) \). Therefore, if we denote \( \sin^2 \alpha \) by \( y \), \( (5) \) becomes a quadratic equation in...
\[ 4y(1 - y) = \frac{1 + y^2}{2}. \]

Solving this equation gives \( y = \frac{4 + \sqrt{7}}{9} \) and \( 4y(1 - y) = \frac{52 + 4\sqrt{7}}{81} = 0.7726\ldots \)

(2) \( \alpha < \beta \).

We consider \( \min(\|P_r(v_1)\|^2 + p_2, 1 - p_2) = \min(\sin^2 \alpha \cos^2 \beta + p_2, 1 - p_2) \).

Since the minimum of two quantities is at most their average, this is at most
\[ \frac{1 + \sin^2 \alpha \cos^2 \beta}{2}. \] (6)

Since \( \alpha < \beta \), we have \( \sin \alpha < \sin \beta \) and (6) is at most \( \frac{1 + \sin^2 \beta \cos^2 \beta}{2} \). This is maximized by \( \sin^2 \beta = 1/2 \). Then, we get \( \frac{1 + 1/4}{2} = \frac{5}{8} \), which is less than \( p = 0.7726\ldots \) which we got in the first case.

This proves the first part of the theorem. \( \square \)

**Construction of a QFA.**

This part is proven by taking the solution of optimization problem 1 and using it to construct a QFA for the language \( a^+ \) in a two-letter alphabet \( \{a, b\} \). The state \( q_1 \) is just the starting state of the minimal automaton, \( q_2 \) is the state to which it gets after reading \( a \), \( x = a \), \( y \) is the empty word and \( z = b \).

Let \( \alpha \) be the solution of (5). Then, \( \sin^2 \alpha = \frac{4 + \sqrt{7}}{9}, \cos^2 \alpha = 1 - \sin^2 \alpha = \frac{5 - \sqrt{7}}{9}, \cos 2\alpha = \cos^2 \alpha - \sin^2 \alpha = \frac{1 - 2\sqrt{7}}{9}, \cos^2 2\alpha = \frac{29 - 4\sqrt{7}}{81} \). \( \sin^2 2\alpha = 1 - \cos^2 2\alpha = \frac{52 + 4\sqrt{7}}{81} \). \( \sin^2 2\alpha \) is the probability of correct answer for our QFA described below.

The QFA \( M \) has 5 states: \( q_0, q_1, q_{\text{acc}}, q_{\text{rej}} \) and \( q_{\text{rej}1} \). \( Q_{\text{acc}} = \{q_{\text{acc}}\}, \) \( Q_{\text{rej}} = \{q_{\text{rej}}, q_{\text{rej}1}\} \). The initial state is \( \sin \alpha |q_0\rangle + \cos \alpha |q_1\rangle \). The transition function is
\[ V_a(|q_0\rangle) = |q_0\rangle, V_a(|q_1\rangle) = \sqrt{\frac{1 + \sin^2 \alpha}{2}} |q_{\text{acc}}\rangle + \frac{\cos \alpha}{\sqrt{2}} |q_{\text{rej}}\rangle; \]
\[ V_b(|q_0\rangle) = |q_{\text{rej}}\rangle, V_b(|q_1\rangle) = |q_{\text{rej}1}\rangle; \]
\[ V_\$ (|q_0\rangle) = \sin \alpha |q_{\text{acc}}\rangle + \cos \alpha |q_{\text{rej}}\rangle, V_\$(|q_1\rangle) = -\cos \alpha |q_{\text{acc}}\rangle + \sin \alpha |q_{\text{rej}}\rangle. \]

To recognize \( L \), \( M \) must accept all words of the form \( a^i \) for \( i > 0 \) and reject the empty word and any word that contains the letter \( b \).

(1) The empty word.
The only transformation applied to the starting state is $V_s$. Therefore, the final superposition is

$$V_s(\sin \alpha |q_0 \rangle + \cos \alpha |q_1 \rangle) = (\sin^2 \alpha - \cos^2 \alpha) |q_{\text{acc}} \rangle + 2 \sin \alpha \cos \alpha |q_{\text{rej}} \rangle.$$ 

The amplitude of $|q_{\text{rej}} \rangle$ in the final superposition is $2 \sin \alpha \cos \alpha = \sin 2\alpha$ and the word is rejected with a probability $\sin^2 2\alpha = 0.772...$.

(2) $a^i$ for $i > 0$.

First, $V_a$ maps the $\cos |q_1 \rangle$ component to

$$\cos \alpha \sqrt{\frac{1 + \sin^2 \alpha}{2}} |q_{\text{acc}} \rangle + \frac{\cos^2 \alpha}{\sqrt{2}} |q_{\text{rej}} \rangle.$$ 

The probability of accepting at this point is $\cos^2 \alpha \frac{1 + \sin^2 \alpha}{2}$. The other component of the superposition, $\sin \alpha |q_0 \rangle$ stays unchanged until $V_s$ maps it to

$$\sin^2 \alpha |q_{\text{acc}} \rangle + \sin \alpha \cos \alpha |q_{\text{rej}} \rangle.$$ 

The probability of accepting at this point is $\sin^4 \alpha$. The total probability of accepting is

$$\cos^2 \alpha \frac{1 + \sin^2 \alpha}{2} + \sin^4 \alpha = (1 - \sin^2 \alpha) \frac{1 + \sin^2 \alpha}{2} + \sin^4 \alpha = \frac{1 + \sin^4 \alpha}{2}.$$ 

By equation (6), this is equal to $\sin^2 2\alpha$.

(3) A word containing at least one $b$.

If $b$ is the first letter of the word, the entire superposition is mapped to rejecting states and the word is rejected with probability 1. Otherwise, the first letter is $a$, it maps $\cos \alpha |q_1 \rangle$ to $\cos \alpha \sqrt{\frac{1 + \sin^2 \alpha}{2}} |q_{\text{acc}} \rangle + \frac{\cos^2 \alpha}{\sqrt{2}} |q_{\text{rej}} \rangle$. The probability of accepting at this point is $\cos^2 \alpha (1 + \sin^2 \alpha)/2 = (1 - \sin^2 \alpha) (1 + \sin^2 \alpha)/2 = (1 - \sin^4 \alpha)/2$. By equation (6), this is the same as $1 - \sin^2 2\alpha$. After that, the remaining component ($\sin \alpha |q_0 \rangle$) is not changed by next $a$s and mapped to a rejecting state by the first $b$. Therefore, the total probability of accepting is also $1 - \sin^2 2\alpha$ and the correct answer (rejection) is given with a probability $\sin^2 2\alpha$.

\[\square\]

4 Non-reversible constructions

We now look at fragments of the minimal automaton that imply that a language cannot be recognized with probability more than $p$, for some $p$. We call such fragments “non-reversible constructions”. The simplest such construction
is the one of Theorem 4. In this section, we present 3 other “non-reversible constructions” that imply that a language can be recognized with probability at most 0.7324..., 0.6894... and $k/(2k-1)$. This shows that different constructions are “non-reversible” to different extent. Comparing these 4 “non-reversible” constructions helps to understand what makes one of them harder for QFA (i.e., recognizable with worse probability of correct answer).

4.1 “Two cycles in a row”

The first construction comes from the language $a^*b^*$ considered in Ambainis and Freivalds [AF 98]. This language was the first example of a language that can be recognized by a QFA with some probability (0.6822...) but not with another $(7/9 + \epsilon)$. We find the “non-reversible” construction for this language and construct the QFA with the best possible accepting probability.

**Theorem 6** Let $L$ be a language and $M$ its minimal automaton.

(1) If $M$ contains states $q_1$, $q_2$ and $q_3$ such that, for some words $x$ and $y$,

(a) if $M$ reads $x$ in the state $q_1$, it passes to $q_1$,
(b) if $M$ reads $y$ in the state $q_1$, it passes to $q_2$,
(c) if $M$ reads $y$ in the state $q_2$, it passes to $q_2$,
(d) if $M$ reads $x$ in the state $q_2$, it passes to $q_3$,
(e) if $M$ reads $x$ in the state $q_3$, it passes to $q_3$

then $L$ cannot be recognized by a QFA with probability more than 0.6894....

(2) The language $a^*b^*$ (the minimal automaton of which contains the construction above) can be recognized by a QFA with probability 0.6894....

**Proof.** By a reduction to the following optimization problem.

**Optimization problem 2.** Find the maximum $p$ such that there is a finite-dimensional space $E$, subspaces $E_a$, $E_r$ such that $E = E_a \oplus E_r$, vectors $v_1$, $v_2$ and $v_3$ and probabilities $p_{a_1}$, $p_{r_1}$, $p_{a_2}$, $p_{r_2}$ such that

(1) $\|v_1 + v_2 + v_3\| = 1$,
(2) $v_1 \perp v_2$,
(3) $v_1 + v_2 + v_3 \perp v_2$,
(4) $v_1 + v_2 \perp v_3$,
(5) $\|v_3\|^2 = p_{a_1} + p_{r_1}$.
(6) $\|v_2\|^2 = p_{a_2} + p_{r_2}$;
(7) $\|P_a(v_1 + v_2 + v_3)\|^2 \geq p$;
(8) $\|P_a(v_1 + v_2)\|^2 + p_{a_1} \geq p$;
(9) $\|P_a(v_1)\|^2 + p_{a_1} + p_{a_2} \leq 1 - p$.

We use a theorem from [BP 99].

**Theorem 7** Let $L$ be a language and $M$ be its minimal automaton. Assume that there is a word $x$ such that $M$ contains states $q_1$, $q_2$ satisfying:

(1) $q_1 \neq q_2$,
(2) If $M$ starts in the state $q_1$ and reads $x$, it passes to $q_2$,
(3) If $M$ starts in the state $q_2$ and reads $x$, it passes to $q_2$, and
(4) There is a word $y$ such that if $M$ starts in $q_2$ and reads $y$, it passes to $q_1$,

then $L$ cannot be recognized by any 1-way quantum finite automaton.

Let $Q$ be a QFA recognizing $L$. Let $q_1$ be state where the minimal automaton $M$ goes if it reads $y$ in the state $q_3$. In case when $q_2 = q_1$ we get the forbidden construction of Theorem 7. In case when $q_2 \neq q_4$ states $q_2$ and $q_4$ are different states of the minimal automaton $M$. Therefore, there is a word $z$ that is accepted in one of them but not in the other. Without loss of generality, we assume that $y$ is accepted if $M$ is started in $q_2$ but not if $M$ is started in $q_4$.

We choose $E_a$ so that the square of the projection $P_a$ of a vector $v$ on $E_a$ is equal to the accepting probability of $Q$ if we run $Q$ on the starting state $v$ and input $yz$ and the right endmarker $\$.

We use Lemma 1. Let $E^x_1$ be $E_1$ and $E^x_2$ be $E_2$ for word $x$ and let $E^y_1$ be $E_y$ and $E^y_2$ be $E_y$ for word $y$.

Without loss of generality we can assume that $q_1$ is a starting state of $M$. Let $\psi_\kappa$ be the starting superposition for $Q$. We can also assume that reading $x$ in this state does not decrease the norm of this superposition. We divide $\psi_\kappa$ into three parts: $v_1$, $v_2$ and $v_3$ so that $v_1 + v_2 \in E^y_1$ and $v_3 \in E^y_2$, $V_1 \in E^x_1$ and $v_2 \in E^x_2$. Due to $v_1 + v_2 + v_3$ is the starting superposition we have $\|v_1 + v_2 + v_3\| = 1$ (Condition 1).

Since $v_1 + v_2 + v_3 \in E^x_1$ we get that $v_1 + v_2 + v_3 \perp v_2$ (Condition 3) due to $v_2 \in E^x_2$. Similarly $v_1 + v_2 \perp v_3$ (Condition 4) and $v_1 \perp v_2$ (Condition 2).

It is easy to get that $\|P_a(v_1 + v_2 + v_3)\|^2 \geq p$ (Condition 7) because reading $yz$ in the state $q_1$ leads to accepting state.

Let $p_{a_1}(p_{r_1})$ be the accepting(rejecting) probability while reading an infinite sequence of letters $y$ in the state $v_1 + v_2 + v_3$. Then $p_{a_1} + p_{r_1} = \|v_3\|^2$ (Condition
5) due to $v_1 + v_2 \in E_1^\eta$ and $v_3 \in E_2^\eta$.

Let $p_{a_2}(p_{r_2})$ be the accepting(rejecting) probability while reading an infinite sequence of letters $x$ in the state $v_1 + v_2$. Then $p_{a_2} + p_{r_2} = \|v_2\|^2$ (Condition 6) due to $v_1 \in E_1^\xi$ and $v_2 \in E_2^\xi$.

We find an integer $i$ such that after reading $y^i$ the norm of $\psi_{xy^i} - (v_1 + v_2)$ is at most some fixed $\epsilon > 0$. Now similarly to Theorem 5 we can get Condition 8: $\|P_a(v_1 + v_2)\|^2 + p_{a_1} \geq p$.

Let $\psi_{xy^i} = \psi_1 + \psi_2$, $\psi_1 \in E_1^\xi$, $\psi_2 \in E_2^\xi$. We find an integer $j$ such that after reading $x^j$ the norm of $\psi_{xy^ix^j} - \psi_1$ is at most $\epsilon$. Since $\psi_1 - v_1 \perp \psi_2 - v_2$ then $\|\psi_1 - v_1\|^2 + \|\psi_2 - v_2\|^2 = \|\psi_{xy^i} - (v_1 + v_2)\|^2 < \epsilon^2$. Therefore, $\|\psi_1 - v_1\| < \epsilon$. Then $\|\psi_{xy^ix^j} - \psi_1\| \leq \|\psi_{xy^ix^j} - \psi_1\| + \|\psi_1 - v_1\| < 2\epsilon$ due to previous inequalities. Now similarly to Theorem 5 we can get Condition 9: $\|P_a(v_1)\|^2 + p_{a_1} + p_{a_2} \leq 1 - p$.

We have constructed our second optimization problem. We solve the problem by computer. Using this solution we can easily construct corresponding quantum automaton. \hfill $\blacksquare$

4.2 $k$ cycles in parallel

**Theorem 8** Let $k \geq 2$.

(1) Let $L$ be a language. If there are words $x_1, x_2, \ldots, x_k$ such that its minimal automaton $M$ contains states $q_0, q_1, \ldots, q_k$ satisfying:

(a) if $M$ starts in the state $q_0$ and reads $x_i$, it passes to $q_i$,
(b) if $M$ starts in the state $q_i (i \geq 1)$ and reads $x_j$, it passes to $q_i$,
(c) for each $i$ the state $q_i$ is not “all-rejecting” state,

Then $L$ cannot be recognized by a QFA with probability greater than $\frac{k}{2k-1}$.

Fig. 3. “The forbidden construction” of Theorem 8.
There is a language such that its minimal deterministic automaton contains this construction and the language can be recognized by a QFA with probability \( \frac{k}{2k-1} \).

For \( k = 2 \), a related construction was considered in [AKV 01]. There is a subtle difference between the two constructions (the one considered here for \( k = 2 \) and the one in [AKV 01]). The “non-reversible construction” in [AKV 01] requires the sets of words accepted from \( q_1 \) and \( q_2 \) to be incomparable. This extra requirement makes it much harder: no QFA can recognize a language with the “non-reversible construction” of [AKV 01] even with the probability \( \frac{1}{2} + \epsilon \).

Proof.

**Impossibility result.** This is the only proof in this paper that does not use a reduction to an optimization problem. Instead, we use a variant of the classification of states (Lemma 2) directly.

We only consider the case when the sets of words accepted from \( q_i \) and \( q_j \) are not incomparable. (The other case follows from the impossibility result in [AKV 01].)

Let \( L_i \) be the set of words accepted from \( q_i (i \geq 1) \). This means that for each \( i, j \) we have either \( L_i \subseteq L_j \) or \( L_j \subseteq L_i \). Without loss of generality we can assume that \( L_1 \subseteq L_2 \subseteq \ldots \subseteq L_k \). Now we can choose \( k \) words \( z_1, z_2, \ldots, z_k \) such that \( z_i \in L_1, L_2, \ldots, L_{k+1-i} \) and \( z_i \notin L_{k+2-i}, \ldots, L_k \). The word \( z_1 \) exists due to the condition (c).

We use a generalization of Lemma 2.

**Lemma 9** Let \( x_1, \ldots, x_k \in \Sigma^+ \). There are subspaces \( E_1, E_2 \) such that \( E_{non} = E_1 \oplus E_2 \) and

1. If \( \psi \in E_1 \), then \( V'_{x_1} (\psi) \in E_1, \ldots, V'_{x_k} (\psi) \in E_1 \) and \( \| V'_{x_1} (\psi) \| = \| \psi \|, \ldots \), \( \| V'_{x_k} (\psi) \| = \| \psi \| \),
2. If \( \psi \in E_2 \), then for any \( \epsilon > 0 \), there exists a word \( t \in (x_1|\ldots|x_k)^* \) such that \( \| V'_t (\psi) \| < \epsilon \).

The proof is similar to lemma 2.

Let \( L \) be a language such that its minimal automaton \( M \) contains the "non-reversible construction" from Theorem 8 and \( M_q \) be a QFA. Let \( p \) be the accepting probability of \( M_q \). We show that \( p \leq \frac{k}{2k-1} \).

Let \( w \) be a word such that after reading it \( M \) is in the state \( q_0 \). Let \( \psi_w = \psi^1_w + \psi^2_w \), \( \psi^1_w \in E_1, \psi^2_w \in E_2 \). We find a word \( a_1 \in (x_1|\ldots|x_k)^* \) such that after
Because of unitarity of $V_{x_1} \ldots V_{x_k}$ on $E_1$ (part (i) of Lemma 9), there exist integers $i_1 \ldots i_k$ such that $\|\psi_{w(x_1a_1)}^{i_1}\| \leq \epsilon, \ldots, \|\psi_{w(x_ka_k)}^{i_k}\| \leq \epsilon$.

Let $p_w$ be the probability of $M_q$ accepting while reading $kw$. Let $p_1, \ldots, p_k$ be the probabilities of accepting while reading $(x_1a_1)^{i_1}, \ldots, (x_ka_k)^{i_k}$ with a starting state $\psi_w$ and and $p'_1, \ldots, p'_k$ be the probabilities of accepting while reading $z_1\$, \ldots, $z_k\$ with a starting state $\psi_w$.

Let us consider $2k - 1$ words:

$kw(x_1a_1)^{i_1}z_k\$, 
$kw(x_2a_2)^{i_2}z_{k-1}\$, 
$kw(x_3a_3)^{i_3}z_{k-1}\$, 
$\ldots$, 
$kw(x_{k-1}a_{k-1})^{i_{k-1}}z_{2}\$, 
$kw(x_ka_k)^{i_k}z_{2}\$, 
$kw(x_ka_k)^{i_k}z_{1}\$.

**Lemma 10** $M_q$ accepts $kw(x_1a_1)^{i_1}z_k\$ with probability at least $p_w + p_1 + p'_k - 4\epsilon$ and at most $p_w + p_1 + p'_k + 4\epsilon$.

**Proof.** The probability of accepting while reading $kw$ is $p_w$. After that, $M_q$ is in the state $\psi_w$ and reading $(x_1a_1)^{i_1}$ in this state causes it to accept with probability $p_1$.

The remaining state is $\psi_{w(x_1a_1)}^{i_1} = \psi_{w(x_1a_1)}^{i_1} + \psi_{w(x_1a_1)}^{2}$. If it was $\psi_{w}^{i_1}$, the probability of accepting while reading the rest of the word ($z_k\$) would be exactly $p'_k$. It is not quite $\psi_{w}^{i_1}$ but it is close to $\psi_{w}^{i_1}$. Namely, we have

$$\|\psi_{w(x_1a_1)}^{i_1} - \psi_{w}^{i_1}\| \leq \|\psi_{w(x_1a_1)}^{2}\| + \|\psi_{w(x_1a_1)}^{i_1} - \psi_{w}^{i_1}\| \leq \epsilon + \epsilon = 2\epsilon.$$

By Lemma 3, this means that the probability of accepting during $z_k\$ is between $p'_k - 4\epsilon$ and $p'_k + 4\epsilon$. □

This Lemma implies that $p_w + p_1 + p'_k + 4\epsilon \geq p$ because of $x_1z_k \in L$. Similarly, $1 - p_w - p_2 - p'_k + 4\epsilon \geq p$ because of $x_2z_k \notin L$. Finally, we have $2k - 1$ inequalities:

$$p_w + p_1 + p'_k + 4\epsilon \geq p,$$
$$1 - p_w - p_2 - p'_k + 4\epsilon \geq p,$$
$$p_w + p_2 + p'_{k-1} + 4\epsilon \geq p,$$
$$1 - p_w - p_3 - p'_{k-1} + 4\epsilon \geq p.$$
\[ \ldots, \\
p_w + p_{k-1} + p'_2 + 4\epsilon \geq p, \\
1 - p_w - p_k - p'_2 + 4\epsilon \geq p, \\
p_w + p_k + p'_1 + 4\epsilon \geq p. \]

By adding up these inequalities we get
\[ k-1 + p_w + p_1 + p'_1 + 4(2k-1)\epsilon \geq (2k-1)p. \]
We can notice that \( p_w + p_1 + p'_1 \leq 1. \) (This is due to the facts that \( p_1 \leq ||\psi_w||^2 \), \( p'_1 \leq ||\psi_w||^2 \) and \( 1 - p_w \leq ||\psi_w||^2 = ||\psi_w||^2 + ||\psi'_w||^2 \). Hence, \( p \leq \frac{k}{2k-1} + 4\epsilon. \)

Since such \( 2k - 1 \) words can be constructed for arbitrarily small \( \epsilon \), this means that \( M_q \) does not recognize \( L \) with probability greater than \( \frac{k}{2k-1} \). \( \square \)

**Constructing a quantum automaton.**

We consider a language \( L_1 \) in the alphabet \( b_1, b_2, \ldots, b_k, z_1, z_2, \ldots, z_k \) such that its minimal automaton has accepting states \( q_0, q_1, \ldots, q_k \) and rejecting state \( q_{\text{rej}} \) and the transition function \( V_1 \) is defined as follows:

\[
V_1(q_0, b_i) = q_i, \quad V_1(q_0, z_i) = q_1, \quad V_1(q_i, b_j) = q_i(i > 1), \quad V_1(q_i, z_j) = q_1(i + j \leq k + 1), \quad V_1(q_i, z_j) = q_{\text{rej}}(i + j > k + 1), \quad V_1(q_{\text{rej}}, b_i) = q_{\text{rej}}, \quad V_1(q_{\text{rej}}, z_i) = q_{\text{rej}}.
\]

It can be checked that this automaton contains the "non reversible construction" from Theorem 4. Hence, this language cannot be recognized by a QFA with probability greater than \( \frac{k}{2k-1} \).

Next, we construct a QFA \( M_q \) that accepts this language with such probability.

The automaton has \( 3(k+1) \) states: \( q'_0, q'_2, \ldots, q'_k, q_{a0}, q_{a2}, \ldots, q_{ak}, q_{r0}, q_{r2}, \ldots, q_{rk} \). \( Q_{\text{acc}} = \{q_{a0}, q_{a2}, \ldots, q_{ak}\}, \) \( Q_{\text{rej}} = \{q_{r0}, q_{r2}, \ldots, q_{rk}\} \). The initial state is

\[
\sqrt{\frac{k}{2k-1}}|q'_0\rangle + \sqrt{\frac{1}{2k-1}}|q'_2\rangle + \ldots + \sqrt{\frac{1}{2k-1}}|q'_k\rangle.
\]

The transition function is

\[
V_{b_i}(|q'_0\rangle) = \sqrt{\frac{k + 1 - i}{k}}|q_{a0}\rangle + \sqrt{\frac{i - 1}{k}}|q_{r0}\rangle, \quad V_{b_i}(|q'_j\rangle) = |q'_j\rangle(j \geq 2),
\]

\[
V_{z_i}(|q'_0\rangle) = |q_{a0}\rangle, \quad V_{z_i}(|q'_j\rangle) = |q_{aj}\rangle(i + j \leq k + 1), \quad V_{z_i}(|q'_j\rangle) = |q_{rj}\rangle(i + j > k + 1), \quad V_{s}(|q'_j\rangle) = |q_{aj}\rangle.
\]

1. The empty word.

The only tranformation applied to the starting state is \( V_s \). Therefore, the final superposition is

\[
\sqrt{\frac{k}{2k-1}}|q_{a0}\rangle + \sqrt{\frac{1}{2k-1}}|q_{a2}\rangle + \ldots + \sqrt{\frac{1}{2k-1}}|q_{ak}\rangle.
\]
and the word is accepted with probability 1.

(2) The word starts with $z_i$.

Reading $z_i$ maps $|q_0\rangle$ to $|q_{a_0}\rangle$. Therefore, this word is accepted with probability at least $(\frac{\sqrt{k^2}}{2k-1})^2 = \frac{k^2}{2k-1}$.

(3) Word is in form $b_i(b_1 \lor \ldots \lor b_k)^*$. The superposition after reading $b_i$ is

$$\sqrt{\frac{k+1-i}{2k-1}}|q_{a_0}\rangle + \sqrt{\frac{i-1}{2k-1}}|q_{r_0}\rangle + \sqrt{\frac{1}{2k-1}}|q'_2\rangle + \ldots + \sqrt{\frac{1}{2k-1}}|q'_{k}\rangle.$$ 

At this moment $M_q$ accepts with probability $\frac{k+i-1}{2k-1}$ and rejects with probability $\frac{i-1}{2k-1}$. The computation continues in the superposition

$$\sqrt{\frac{1}{2k-1}}|q'_2\rangle + \ldots + \sqrt{\frac{1}{2k-1}}|q'_{k}\rangle.$$ 

Clearly, that reading of all remaining letters does not change this superposition. Since $V_S$ maps each $|q'_j\rangle$ to an accepting state then $M_q$ rejects this word with probability at most $\frac{i-1}{2k-1} \leq \frac{k-1}{2k-1}$.

(4) Word $x$ starts with $b_i(b_1 \lor \ldots \lor b_k)^*z_j$. Before reading $z_j$ the superposition is

$$\sqrt{\frac{1}{2k-1}}|q'_2\rangle + \ldots + \sqrt{\frac{1}{2k-1}}|q'_{k}\rangle.$$ 

Case 1. $i+j > k+1$. $x \notin L_1$.

Since $i+j > k+1$ then reading $z_j$ maps at least $k-i+1$ states of $q'_2, \ldots, q'_k$ to rejecting states. This means that $M_q$ rejects with probability at least

$$\frac{i-1}{2k-1} + \frac{k-i+1}{2k-1} = \frac{k}{2k-1}.$$ 

Case 2. $i+j \leq k+1$. $x \in L_1$. Since $i+j \leq k+1$ then reading $z_j$ maps at least $i-1$ states of $q'_2, \ldots, q'_k$ to accepting states. This means that $M_q$ accepts with probability at least

$$\frac{k+1-i}{2k-1} + \frac{i-1}{2k-1} = \frac{k}{2k-1}.$$ 

$\square$

4.3 0.7324... construction

**Theorem 11** Let $L$ be a language.

(1) If there are words $x, z_1, z_2$ such that its minimal automaton $M$ contains states $q_1$ and $q_2$ satisfying:

(a) if $M$ starts in the state $q_1$ and reads $x$, it passes to $q_2$, 

(b) if $M$ starts in the state $q_2$ and reads $x$, it passes to $q_2$,
(c) if $M$ starts in the state $q_1$ and reads $z_1$, it passes to an accepting state,
(d) if $M$ starts in the state $q_1$ and reads $z_2$, it passes to a rejecting state,
(e) if $M$ starts in the state $q_2$ and reads $z_1$, it passes to a rejecting state,
(f) if $M$ starts in the state $q_2$ and reads $z_2$, it passes to an accepting state.

Then $L$ cannot be recognized by a QFA with probability greater than $\frac{1}{2} + \frac{3\sqrt{15}}{50} = 0.7324$.

(2) There is a language $L$ with the minimum automaton containing this construction that can be recognized with probability $\frac{1}{2} + \frac{3\sqrt{15}}{50} = 0.7324$.

Proof.

Impossibility result.

The construction of optimization problem is similar to the construction of Optimization problem 1. For this reason, we omit it and just give the optimization problem and show how to solve it.

Optimization problem 3. Find the maximum $p$ such that there is a finite dimensional vector space $E_{opt}$, subspaces $E_a$, $E_r$ (unlike in previous optimization problems, $E_a$ and $E_r$ do not have to be orthogonal) and vectors $v_1$, $v_2$ such that $v_1 \perp v_2$ and $\|v_1 + v_2\|^2 = 1$ and probabilities $p_1$, $p_2$ such that $p_1 + p_2 = \|v_2\|^2$ and

1. $\|P_a(v_1 + v_2)\|^2 \geq p$,
2. $\|P_r(v_1 + v_2)\|^2 \geq p$,
3. $1 - \|P_a(v_1)\|^2 - p_1 \geq p$,
4. $1 - \|P_r(v_1)\|^2 - p_2 \geq p$.

Solving optimization problem 3.

Without loss of generality we can assume that $\|P_a(v_1)\| \leq \|P_r(v_1)\|$. Then these four inequalities can be replaced with only three inequalities

1. $\|P_a(v_1 + v_2)\|^2 \geq p$,
2. $1 - \|P_a(v_1)\|^2 - p_1 \geq p$,
(3) \(1 - \|P_a(v_1)\|^2 - p_2 \geq p\).

Clearly that \(p\) is maximized by \(p_1 = p_2 = \frac{\|v_2\|^2}{2}\). Therefore, we have

\[
\begin{align*}
(1) & \quad \|P_a(v_1 + v_2)\|^2 \geq p, \\
(2) & \quad 1 - \|P_a(v_1)\|^2 - \frac{\|v_2\|^2}{2} \geq p.
\end{align*}
\]

Next we show that it is enough to consider only instances of small dimension. We denote \(E_{opt} - E_a\) as \(E_b\). First, we restrict \(E_a\) to the subspace \(E'_a\) generated by projections of \(v_1\) and \(v_2\) to \(E_a\). This subspace is at most 2-dimensional. Similarly, we restrict \(E_b\) to the subspace \(E'_b\) generated by projections of \(v_1\) and \(v_2\) to \(E_b\). The lengths of all projections are still the same. We fix an orthonormal basis for \(E_{opt}\) so that \(P_a(v_1)\) and \(P_b(v_1)\) are both parallel to some basis vectors. Then, \(v_1 = (x_1, 0, x_3, 0)\) and \(v_2 = (y_1, y_2, y_3, y_4)\) where the first two coordinates correspond to basis vectors of \(E'_a\) and the last two coordinates correspond to basis vectors of \(E'_b\). We can assume that \(x_1\) and \(x_3\) are both non-negative. (Otherwise, just invert the direction of one of basis vectors.)

Let \(\Delta = \|v_1\| = \sqrt{x_1^2 + x_3^2}\). Then, there is \(\alpha \in [0, \pi/2]\) such that \(x_1 = \Delta \cos \alpha\), \(x_3 = \Delta \sin \alpha\). Let \(\delta = \sqrt{y_1^2 + y_3^2}\). Then, \(y_1 = \delta \sin \alpha\), \(y_3 = -\delta \cos \alpha\) because \(x_1 y_1 + x_3 y_3 = 0\) due to \(v_1 \perp v_2\). If \(y_4 \neq 0\), we can change \(y_1\) and \(y_3\) to \(\delta' \sin \alpha\) and \(-\delta' \cos \alpha\) where \(\delta' = \sqrt{y_1^2 + y_3^2 + y_4^2}\) and this only increases \(\|P_a(v_1 + v_2)\|\). Hence, we can assume that \(y_4 = 0\). We denote \(\epsilon = y_2\). Then, \(v_1 = (\Delta \cos \alpha, 0, \Delta \sin \alpha, 0), v_2 = (\delta \sin \alpha, \epsilon, -\delta \cos \alpha, 0)\).

Let \(E = \sqrt{\Delta^2 + \delta^2}\). Then, \(\Delta = E \sin \beta\) and \(\delta = E \cos \beta\) for some \(\beta \in [0, \pi/2]\) and \(E^2 + \epsilon^2 = 1\). This gives

\[
\begin{align*}
(1) & \quad \|P_a(v_1 + v_2)\|^2 = E^2(\sin \beta \cos \alpha + \cos \beta \sin \alpha)^2 + \epsilon^2 = E^2 \sin^2(\alpha + \beta) + \epsilon^2 \geq p, \\
(2) & \quad 1 - \|P_a(v_1)\|^2 - \frac{\|v_2\|^2}{2} = 1 - E^2 \sin^2 \beta \cos^2 \alpha - \frac{E^2 \cos^2 \beta + \epsilon^2}{2} \geq p.
\end{align*}
\]

Then after some calculations we get

\[
\begin{align*}
(1) & \quad 1 - E^2 \cos^2 (\alpha + \beta) \geq p, \\
(2) & \quad \frac{1 - E^2 \sin^2 \beta \cos 2\alpha}{2} \geq p.
\end{align*}
\]

If we fix \(\alpha + \beta\) and vary \(\beta\), then \(-\sin^2 \beta \cos 2\alpha\) (and, hence, \(\frac{1 - E^2 \sin^2 \beta \cos 2\alpha}{2}\)) is maximized by \(\beta = 2\alpha - \pi/2\). This means that we can assume \(\beta = 2\alpha - \pi/2\) and we have

\[
\begin{align*}
(1) & \quad 1 - E^2 \sin^2 (3\alpha) \geq p, \\
(2) & \quad \frac{1 - E^2 \cos^3 (2\alpha)}{2} \geq p.
\end{align*}
\]

If we consider \(\cos^2 \alpha \geq 1/2\) then \(p \leq \frac{1 - E^2 \cos^3 (2\alpha)}{2} = \frac{1 - E^2 (2 \cos^2 \alpha - 1)^3}{2} \leq 1/2\). This means that we are only interested in \(\cos^2 \alpha < 1/2\).
Let \( f(E^2, \alpha) = 1 - E^2 \sin^2(3\alpha) \) and \( g(E^2, \alpha) = \frac{1 - E^2 \cos^3(2\alpha)}{2} \). If we fix \( \alpha \) and vary \( E^2 \), then \( f \) and \( g \) are linear functions in \( E^2 \) and \( f(0, \alpha) > g(0, \alpha) \). We consider two cases.

Case 1. \( f(1, \alpha) \geq g(1, \alpha) \). (This gives \( f(E^2, \alpha) \geq g(E^2, \alpha) \) for each \( E^2 \). Therefore, in this case we only need to maximize the function \( g \).

This means that
\[
1 - \sin^2(3\alpha) \geq \frac{1 - \cos^3(2\alpha)}{2},
\]
\[
1 - 2\sin^2(3\alpha) + \cos^3(2\alpha) \geq 0,
\]
\[
1 - 2(1 - \cos^2(3\alpha)) + \cos^3(2\alpha) \geq 0,
\]
\[
1 - 2(1 - (4\cos^3\alpha - 3\cos\alpha)^2) + \cos^3(2\alpha) \geq 0,
\]
\[
1 - 2(1 - 16\cos^6\alpha + 24\cos^4\alpha - 9\cos^2\alpha + (2\cos^2\alpha - 1)^3 \geq 0,
\]
\[
20\cos^6\alpha - 30\cos^4\alpha + 12\cos^2\alpha - 1 \geq 0,
\]
\[
(1 - 2\cos^2\alpha)(-10\cos^4\alpha + 10\cos^2\alpha - 1) \geq 0.
\]
So that \( \cos^2\alpha < 1/2 \), we have
\[
-10\cos^4\alpha + 10\cos^2\alpha - 1 \geq 0.
\]
This means that \( \cos^2\alpha \in \left[ \frac{1}{2} - \frac{\sqrt{15}}{10}, \frac{1}{2} \right] \).

Since \( g(E^2, \alpha) = \frac{1 - E^2(2\cos^2\alpha - 1)^3}{2} \), \( g \) is maximized by \( E^2 = 1 \) and \( \cos^2\alpha = \frac{1}{2} - \frac{\sqrt{15}}{10} \). This gives \( p \) equal to \( \frac{1}{2} + \frac{3\sqrt{15}}{50} \).

Case 2. \( f(1, \alpha) \leq g(1, \alpha) \). (This is equivalent to \( \cos^2\alpha \in [0, \frac{1}{2} - \frac{\sqrt{15}}{10}] \).)

This means that \( p \) is maximized by \( f(E^2, \alpha) = g(E^2, \alpha) \). Therefore,
\[
(1) \quad 1 - E^2 \sin^2(3\alpha) = p,
\]
\[
(2) \quad \frac{1 - E^2 \cos^3(2\alpha)}{2} = p.
\]

Let \( y = -\cos 2\alpha = 1 - 2\cos^2\alpha \). Then \( y \in [\sqrt{\frac{3}{5}}, 1] \) and \( \sin^2(3\alpha) = 1 - \cos^2(3\alpha) = 1 - (4\cos^3\alpha - 3\cos\alpha)^2 = 1 - \cos^2\alpha(4\cos^2\alpha - 3)^2 = 1 - \frac{1 - y^2}{2}(1 + 2y)^2 = \frac{1 - 3y + 4y^3}{2} \). Therefore,
\[
(1) \quad 2 - E^2(4y^3 - 3y + 1) = 2p,
\]
\[
(2) \quad 1 + E^2y^3 = 2p.
\]

Now we express \( p \) using only \( y \). We get \( p = \frac{1}{2} + \frac{y^3}{2(5y^2 - 3y + 1)} \). Finally, if we vary \( y \) through the interval \( [\sqrt{\frac{3}{5}}, 1] \), then \( p \) is maximized by \( y = \sqrt{\frac{3}{5}} \). This gives \( p \) equal to \( \frac{1}{2} + \frac{3\sqrt{15}}{50} \). □

Construction of a QFA.
We consider the two letter alphabet \( \{a, b\} \). The language \( L \) is the union of the empty word and \( a^+b(a \lor b)^* \). Clearly that the minimal deterministic automaton of \( L \) contains the ”non reversible construction” from Theorem 5 (just take \( a \) as \( x \), the empty word as \( z_1 \) and \( b \) as \( z_2 \)).

Next, we describe a QFA \( M \) accepting this language. Let \( \alpha \) be the solution of \( 1 - 2 \cos^2 \alpha = \sqrt{\frac{3}{5}} \) in the interval \([0, \pi/2]\). It can be checked that \( \cos^2(3\alpha) = \frac{1}{2} + \frac{3\sqrt{15}}{50} \), \( \sin^2 2\alpha = \frac{2}{5} \), \( \cos^2 2\alpha = \frac{3}{5} \), \( \sin^2 \alpha = \frac{1}{2} + \frac{\sqrt{3}}{2\sqrt{5}} \).

The automaton has 4 states: \( q_0, q_1, q_{acc} \) and \( q_{rej} \). \( Q_{acc} = \{q_{acc}\}, Q_{rej} = \{q_{rej}\} \). The initial state is \( \cos(3\alpha)|q_0\rangle + \sin(3\alpha)|q_1\rangle \). The transition function is

\[
V_a(|q_0\rangle) = \cos^2 \alpha |q_0\rangle + \cos \alpha \sin \alpha |q_1\rangle + \frac{\sin \alpha}{\sqrt{2}} |q_{acc}\rangle + \frac{\sin \alpha}{\sqrt{2}} |q_{rej}\rangle,
\]

\[
V_a(|q_1\rangle) = \cos \alpha \sin \alpha |q_0\rangle + \sin^2 \alpha |q_1\rangle - \frac{\cos \alpha}{\sqrt{2}} |q_{acc}\rangle - \frac{\cos \alpha}{\sqrt{2}} |q_{rej}\rangle,
\]

\[
V_b(|q_0\rangle) = |q_{rej}\rangle, V_b(|q_1\rangle) = |q_{acc}\rangle,
\]

\[
V_\$ (|q_0\rangle) = |q_{acc}\rangle, V_\$ (|q_1\rangle) = |q_{rej}\rangle,
\]

(1) The empty word.

The only transformation applied to the starting state is \( V_\$ \). Therefore, the final superposition is \( \cos(3\alpha)|q_{acc}\rangle + \sin(3\alpha)|q_{rej}\rangle \) and the word is accepted with probability \( \cos^2(3\alpha) = \frac{1}{2} + \frac{3\sqrt{15}}{50} \).

(2) \( b(a \lor b)^* \).

After reading \( b \) the superposition is \( \sin(3\alpha)|q_{acc}\rangle + \cos(3\alpha)|q_{rej}\rangle \) and word is rejected with probability \( \cos^2(3\alpha) = \frac{1}{2} + \frac{3\sqrt{15}}{50} \).

(3) \( a^+ \).

After reading the first \( a \) the superposition becomes

\[
\cos \alpha \cos 2\alpha |q_0\rangle + \sin \alpha \cos 2\alpha |q_1\rangle - \frac{\sin 2\alpha}{\sqrt{2}} |q_{acc}\rangle - \frac{\sin 2\alpha}{\sqrt{2}} |q_{rej}\rangle.
\]

At this moment \( M \) accepts with probability \( \frac{\sin^2 2\alpha}{2} = \frac{1}{5} \) and rejects with probability \( \frac{1}{5} \). The computation continues in the superposition

\[
\cos \alpha \cos 2\alpha |q_{acc}\rangle + \sin \alpha \cos 2\alpha |q_{rej}\rangle.
\]

It is easy to see that reading all of remaining letters does not change this superposition.

Therefore, the final superposition (after reading \( \$ \)) is

\[
\cos \alpha \cos 2\alpha |q_{acc}\rangle + \sin \alpha \cos 2\alpha |q_{rej}\rangle.
\]
This means that $M$ rejects with probability

$$\sin^2 \alpha \cos^2 2\alpha + \frac{1}{5} = \frac{3}{5} \left( \frac{1}{2} + \frac{\sqrt{3}}{2\sqrt{5}} \right) + \frac{1}{5} = \frac{1}{2} + \frac{3\sqrt{15}}{50}.$$  

(4) $a^+b(a \lor b)^*$. Before reading the first $b$ the superposition is

$$\cos \alpha \cos 2\alpha |q_0\rangle + \sin \alpha \cos 2\alpha |q_1\rangle$$

and reading this $b$ changes this superposition to

$$\sin \alpha \cos 2\alpha |q_{\text{acc}}\rangle + \cos \alpha \cos 2\alpha |q_{\text{rej}}\rangle.$$  

This means that $M$ accepts with probability

$$\sin^2 \alpha \cos^2 2\alpha + \frac{1}{5} = \frac{1}{2} + \frac{3\sqrt{15}}{50}.$$  

\[\square\]

5 Conclusion

Quantum finite automata (QFA) can recognize all regular languages if arbitrary intermediate measurements are allowed. If they are restricted to be unitary, the computational power drops dramatically, to languages recognizable by permutation automata [CM 97, BP 99]. In this paper, we studied an intermediate case in which measurements are allowed but restricted to ”accept-reject-continue” form (as in [KW 97, AF 98, BP 99]).

Quantum automata of this type can recognize several languages not recognizable by the corresponding classical model (reversible finite automata). In all of those cases, those languages cannot be recognized with probability 1 or $1 - \epsilon$, but can be recognized with some fixed probability $p > 1/2$. This is an unusual feature of this model because, in most other computational models a probability of correct answer $p > 1/2$ can be easily amplified to $1 - \epsilon$ for arbitrary $\epsilon > 0$.

In this paper, we study maximal probabilities of correct answer achievable for several languages. Those probabilities are related to “forbidden constructions” in the minimal automaton. A “forbidden construction” being present in the minimal automaton implies that the language cannot be recognized with a probability higher than a certain $p > 1/2$.  

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The basic construction is “one cycle” in figure 1. Composing it with itself sequentially (figure 2) or in parallel (figure 3) gives “forbidden constructions” with a smaller probability $p$. The achievable probability also depends on whether the sets of words accepted from the different states of the construction are subsets of one another (as in figure 1) or incomparable (as in figure 4). The constructions with incomparable sets usually imply smaller probabilities $p$.

The accepting probabilities $p$ quantify the degree of non-reversibility present in the “forbidden construction”. Lower probability $p$ means that the language is more difficult for QFA and thus, the “construction” has higher degree of non-reversibility. In our paper, we gave a method for calculating this probability and used it to calculate the probabilities $p$ for several “constructions”. The method should apply to a wide class of constructions but solving the optimization problems can become difficult if the construction contains more states (as for language $a_1^*a_2^*\ldots a_k^*$ studied in [ABFK 99]). In this case, it would be good to have methods for calculating the accepting probabilities approximately.

A more general problem suggested by this work is: how do we quantify non-reversibility? Accepting probabilities of QFAs provide one way of comparing the degree of non-reversibility in different “constructions”. What are the other ways of quantifying it? And what are the other settings in which similar questions can be studied?

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