Numerical simulations of mixed states quantum computation

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Abstract

We describe quantum-octave package of functions useful for simulations of quantum algorithms and protocols. Presented package allows to perform simulations with mixed states. We present numerical implementation of important quantum mechanical operations – partial trace and partial transpose. Those operations are used as building blocks of algorithms for analysis of entanglement and quantum error correction codes. Simulation of Shor’s algorithm is presented as an example of package capabilities.

1 Motivation

Most of software developed for simulations of quantum computing is based on finite dimensional Hilbert space formalism. Mixed state model for quantum computing allows to incorporate many features which are crucial for analysis of entanglement and decoherence.

Main contribution of this work is presentation of quantum-octave package – a tool which allows to perform simulations of quantum systems using density operators formalism in convenient way. We present algorithms used in implementation of partial operations in quantum-octave. Sample results obtained using quantum-octave present capabilities of package.

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2 Implementation in GNU Octave language

Package quantum-octave is implemented in GNU Octave language. List of functions and their detailed description can be found on project webpage. We present here only the most important features of quantum-octave.

Most of quantum-octave functions can be applied to density operators, which are represented by normalise matrices. Package offers also functions for operations on pure states. Base ket vectors and their linear combinations are easily constructed and transformed into corresponding density operators using State function, and it is easy to obtain mixtures of states using MixStates function. Computation process is performed using Evolve(gate, state) function, where gate is unitary operation.

Lowlevel functions BinVec2Dec and Dec2BinVec allow for convenient use of register notation (|1⟩ ⊗ |0⟩ ⊗ |0⟩ ⊗ ... ⊗ |0⟩). They are implemented in C++ using liboctave are they are used for manipulations of registers in PTrace and PTranspose functions. For example sequence of operations
\[
y = \text{Dec2BinVec}(3,4);
ymp = y(2);
y(2) = y(3);
y(3) = 
\]
x = Ket(BinVec2Dec(y));

allows to permute second and third qubits in base state in four dimensional space.

3 Algorithms for partial operations

Partial operations are crucial for analysis of quantum information processing. Partial transposition allows to distinguish entangled and separable states in low dimensional systems. This operation was used in Ref. for constructing computable measure of entanglement – negativity.\footnote{Negativity is defined as a sum of negative eigenvalues of density matrix after partial transposition. It is easy to check that this definition is equivalent to formula $N(\rho) = ||\rho^{TA}||_1 - 1$, where $||\rho||_1$ denotes trace norm of density matrix $\rho$.}

3.1 Partial transposition using registers

In quantum-octave partial transposition is based on permutation of qubits indexes. Suppose we perform partial transposition with respect to some
qubits in input state. Let \( Q = \{ q_1, q_2, \ldots, q_n \} \subset \mathbb{N} \) be the set of numbers labelling those qubits. Using register notation one can write
\[
\langle \alpha | \rho^{T_{q_1, \ldots, q_n}} | \beta \rangle = \langle V(\alpha, \beta, q_1, \ldots, q_n) | \rho | V(\beta, \alpha, q_1, \ldots, q_n) \rangle,
\]
where
\[
V_i(\alpha, \beta, q_1, \ldots, q_n) = \begin{cases} 
\beta_i, & i \in \{ q_1, \ldots, q_n \} \\
\alpha_i, & i \notin \{ q_1, \ldots, q_n \}
\end{cases}
\]
and \( \alpha_i, \beta_i, V_i \) represent \( i \)-th number in binary representation of \( \alpha, \beta \) and \( V \).

### 3.2 Partial trace

For density matrix \( \rho \in S(\mathcal{H}_A \otimes \mathcal{H}_B) \) one can obtain description of subsystems \( A \) and \( B \) using partial trace operation.\cite{6} In quantum-octave this operation is implemented as follows. Let \( Q = \{ q_1, q_2, \ldots, q_n \} \) be a given set of number labelling qubits. Density operator describing state of this qubits is defined as matrix with elements
\[
\langle \alpha | tr_{q_1, q_2, \ldots, q_n} (\rho) | \beta \rangle = \sum_{k_1=0}^{1} \cdots \sum_{k_n=0}^{1} \langle W(\alpha, k_1, \ldots, k_n) | \rho | W(\beta, k_1, \ldots, k_n) \rangle,
\]
where \( \alpha \) and \( \beta \) are binary digits of length \( m = N - n \). Number \( k_1, \ldots, k_n \in \{0, 1\} \) label base vectors in Hilbert spaces of qubits \( q_1, \ldots, q_n \) respectively. Numbers \( W \) are constructed as follows
\[
W(\alpha, k_1, \ldots, k_n) = (W_1, W_2, \ldots, W_N), \quad W_i = \begin{cases} 
\alpha_i, & i \in Q \\
k_i, & i \notin Q
\end{cases}
\]
In quantum-octave construction of numbers \( W \) is performed using function \texttt{BuildBinaryVector} implemented in C++. This is motivated by extensive usage of this function. If one wants to perform partial trace operation on \( N \)-qubit system with respect to its \( m \)-qubit subsystem, function \texttt{BuildBinaryVector} have to be called \( 2^{2(N-m)N} \) times.

One should note that this algorithm allows to perform partial trace with respect to any set of qubits.

### 4 Shor’s algorithm with mixed sates – fidelity and distances measures

In this section we present sample results obtained by using quantum-octave. We analyse influence of states mixing on Shor’s algorithm.\footnote{The subject of analysis is restricted to quantum part of Shor’s algorithm.} The idea was
Figure 1: Comparison of distance measures between density matrices (Fig. 1(a)) and between probability distributions (Figs. 1(b)-1(d)) for simulation of Shor’s algorithm to observe how quantum state, obtained by performing quantum algorithm on non-pure state, differs from state obtained in ideal (pure state) case. On each step of simulation Initial state $\rho_p$ was prepared as mixture of pure state $\rho_0 = \sum_{d} |00\ldots0\rangle\langle00\ldots0|$ and maximally mixed state $I_d/d$

$$\rho_p = (1-p)\rho_0 + pI_d/d,$$

(5)
where $p \in \{0.00, 0.01, 0.02, \ldots, 1.00\}$ and $I_d$ is $d$-dimensional identity matrix. For each state obtained in such way the trivial and Shor’s circuits were applied and for each obtained outcome two distances and two fidelity measures were calculated. Results of those simulations are presented in Fig. 1. Shor’s algorithm is performed on 7 qubits, but only the first 3 qubits are taken into account during calculations of fidelity and distance measures because the last 4 qubits decohere and normally aren’t measured.

Fidelity between density matrices, as given in Ref. 6 is proper measure which shows how much two mixed states differ. To compare different methods of calculating distance between states we have chosen three functions (Eqs. 7, 8 and 9) that operate on probability distributions. Probability distributions are obtained by performing measurement of observable $\hat{Z} \otimes \hat{Z} \otimes \hat{Z}$. Formulas used to calculate measures are presented below. Let $p_1, p_2$ be probability distributions, and $\rho_1, \rho_2$ - density matrices.

- Fidelity between density matrices
  \[
  F(\rho_1, \rho_2) = \text{tr} \sqrt{\sqrt{\rho_1} \rho_2 \sqrt{\rho_1}},
  \]

- Fidelity between probability distributions
  \[
  F(p_1, p_2) = \sum_{x \in X} \sqrt{p_1(x)} \sqrt{p_2(x)},
  \]

  where $p = \frac{1}{2}(p_1 + p_2)$;

- $\chi^2$-measure
  \[
  \chi^2(p_1, p_2) = \sum_{x \in X} \frac{(p_1(x) - p(x))^2}{p(x)},
  \]

- Trace-distance
  \[
  F(p_1, p_2) = \frac{1}{2} \sum_{x \in X} |p_1(x) - p_2(x)|.
  \]

One can conclude that for small addition of noise results differs very much from the ideal case. The loss of quality grows slower for bigger contribution of noise.
5 Final remarks

Package quantum-octave allows to perform simulations of mixed states quantum computation in convenient way. It also provides functions for analysis of entanglement and quantum errors. Quantum protocols and algorithm such as teleportation,\[1\] qubit authentication\[2\] or Shor’s algorithm\[9\] can be easily implemented as GNU Octave functions and the use in further simulations. This allows to perform simulations operating on high level quantum primitives (e.g. qubit authentication, error correcting code).

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