Speedup problem for quantum walks and quantum annealing algorithms implementation

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Plan of Talk

- Introduction to Classical Random (CRW) and Quantum Walks (QW)
- Machine Learning approach to speedup problem for Random Walks algorithms
- Results and conclusions
Welcome to Highly Non-classical University!

- 2nd University in Russia and in top 150 of QS WUR in Computer Science & info Systems,
- Seven-time Champions in ICPC,
- 2nd in 5-100 Federal target program ranking for Russian Universities.

RoboCup Open Russia-2019
Classical and quantum walks paradigm

### Classical

-6 -5 -4 -3 -2 -1 0 1 2 3 4 5 6

### Quantum

-6 -5 -4 -3 -2 -1 0 1 2 3 4 5 6

Starting point
Classical random - Galton Board

Quantum walks – Coined QW

Translation operator

\[
S = \sum_{x \in \mathbb{Z}} (|x+1 \rangle \langle x| \otimes \uparrow \langle \uparrow | + |x-1 \rangle \langle x| \otimes |\downarrow \rangle \langle \downarrow |).
\]

The wave packets symbolize the probability Amplitudes for the states to be occupied. The ±-signs correspond to the polarization state. Positive amplitudes are in red color, negative amplitudes are blue.
Experiment on QW with photons

The observed output pattern of light intensity after short (blue) and long (green) propagation in a periodic lattice. This well-known pattern is one of the hallmarks of the ballistic propagation of QWs. (c) Output patterns of light intensity resulting from injection of light into two adjacent single waveguides (sites 42 and 43) of a disordered lattice. The different patterns observed demonstrate the high sensitivity of the QW to the initial conditions in this case.

Quantum (search) algorithms. Speedup is approaches to $O(\sqrt{N})$

Quantum computing
A. M. Childs, PRL 102, 180501 (2009); Science 339, 791 (2013)

Quantum transport in biophotonics (FMO complexes)
M. Mohseni, et al., The J. of chemical physics 129, 174106 (2008)

Quantum AI

Design of new quantum experiments
Classical Random Walks (CRW)

Transition matrix elements that defines dynamics:

\[ T_{ij} = T_{ji} \quad T_{ii} = 0 \] (Without loops)

Let \( \epsilon \) be the probability of elementary transition.

Probability distribution changes as:

\[ p(t) - p(t - 1) = \epsilon (T - I) p(t - 1) \]

Discrete time random walks:

\[ p(t) = Tp(t - 1) \]

Continuous time random walks:

\[ \frac{d}{dt} p(t) = (T - I) p(t) \]
Quantum Random Walks (QW)

\[ H_{ij} \text{ is Hamiltonian matrix elements} \]

\[ H_{ij} = H_{ji}, \quad H_{ii} = 0 \]

Hopping Hamiltonian is

\[ H = \hbar J \sum_{(i,j)} |i\rangle \langle j| \]

Discrete time random walks

\[ H = H_{\text{particle}} \otimes H_{\text{coin}} \]

Shift \[ |x\rangle |\uparrow\rangle = |x+1\rangle |\uparrow\rangle, \]

Shift \[ |x\rangle |\downarrow\rangle = |x-1\rangle |\downarrow\rangle \]

\[ |\psi(t)\rangle = \text{Shift} \left( I \otimes \text{Had} \right) |\psi(t-1)\rangle \]

Continuous time random walks

\[ i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = H |\psi(t)\rangle \]

QW are quadratically faster than CW on:

- line
- glued tries
- hypercube

- is starting point
- Is final point


A. A. Melnikov, A. Alodjants, L. Fedichkin, Hitting time for quantum walks of identical particles, SPIE, 2018
Speedup problem

However!

- Positions of input and output points are important,
- There exist “dark” areas (due to quantum destructive interference) where particle disappear,
- Specifics of quantum measurement.

How we can detect speedup of random walk for arbitrary graph?

Initial vertices

Final vertices

Adjacency (A)- matrix $A_{ij}$

\[
\begin{pmatrix}
0 & 1 & 0 & 0 & 1 & 0 \\
1 & 0 & 1 & 0 & 1 & 0 \\
0 & 1 & 0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 & 1 & 1 \\
1 & 1 & 0 & 1 & 0 & 0 \\
0 & 0 & 0 & 1 & 0 & 0 \\
\end{pmatrix}
\]

We consider:
- Undirected graphs,
- Connective graphs

The On-Line Encyclopedia of Integer Sequences® (OEIS®)

Toy Model of QWs

Simple graph sample on the line

QW

\[ p(t) = e^{(T-I)t} p(0) = e^{-t} e^{Tt} p(0), \]

Corresponding to a classical particle initially located in \( v = 1 \).

CRW

Detection Probability

The Master Equation

\[ \frac{d\rho(t)}{dt} = -\frac{i}{\hbar} [H, \rho(t)] + \gamma \left( L\rho(t)L^\dagger - \frac{1}{2} \{LL^\dagger, \rho(t)\} \right) \]

\[ H = \hbar A^q. \]

\[ A^q \text{ is } (n + 1) \times (n + 1) \text{ matrix} \]

\[ \gamma \text{ characterizes decay from the final state } 2 \text{ to the output ("sink") vertices } 4 \]

\[ L = |n + 1\rangle \langle n| \]
The ML approach for detecting quantum speedup

Training of convolutional neural network

Example of CNN architecture

Testing of convolutional neural network

The number of filters are taken from set of experiences
Filtering

Initial A-matrix

Convolution procedure as usual

Convolutional filters and procedure that we use

Edge to edge filtering

Indicates the number of edge-to-edges

“Halve” of A-matrix
These results are the average over 100 independent CNNs. Losses are defined through cross-entropy.

Accuracy of prediction with test samples

Mean squared deviation is shown as a vertical line for each bar. The zeroth component of the feature vector is the bias. The first feature for each vertex corresponds to the number of edges this vertex has. The second feature to the total number of neighboring edges of all edges leading to the vertex. The third feature gives one if the vertex is connected to the initial vertex by an edge, and zero otherwise. The fourth feature does the same relative to the target vertex.
CNN predictions for large graphs

Classical walker is faster

Quantum walker is faster
Conclusions

- We propose convolutional neural network paradigm for speedup detection of random walks on the graphs,
- Detection is 90% and more for test graphs taken on the line,
- Training in small graphs allowed the neural network to build a model which works on graphs of higher dimension,
- Neural network recognized about 25% of “quantum” graphs using random graphs samples. Moreover, when the network said “quantum”, it was right in 90% cases.

Publications

For quantum annealing pls, look
Thank you for attention!