Responses to Reviewers

on Paper *Beyond Classical Diffusion: Ballistic Graph Neural Network*

Referee #3 and #2:
More experiments to demonstrate the power of ballistic comparing to classical ones.
Classification on different DATASETs(accuracy %)

Name of dataset	Classical Diffusion based ([1])	Classical Diffusion based ([2])	Ballistic (this paper)
CIFAR-10	93.65	93.49	***94.73***
CIFAR-100	60.30	59.51	***61.24***
STL-10	55.28	58.87	***63.32***

[1] Thomas N Kipf and Max Welling. Semi-supervised classification with graph convolutional networks. *arXiv preprint arXiv:1609.02907*, 2016.

[2] Michaël Defferrard, Xavier Bresson, and Pierre Vandergheynst. Convolutional neural networks on graphs with fast localized spectral filtering. In *Advances in neural information processing systems*, pp. 3844–3852, 2016.

Referee #1:

If the contribution is only a new kind of random walk on a graph, is ICLR the good targeted venue ?

Response: Answer: Yes, random walk on graph is a very important problem. In GCN, random walk is the way you collect the information. The traditional pipeline is show attached.

The Feature Extraction lies as the ***cornerstone*** *of the GCN problem:*
For almost all previous papers, the methods used are based on a random walk (Laplacian matrix), resulting in the over-smooth problem as **Referee #3** *mentioned. The method we propose in this paper is inspired by quantum diffusion and is completely different from the previous one. Our method also achieves better performance.*

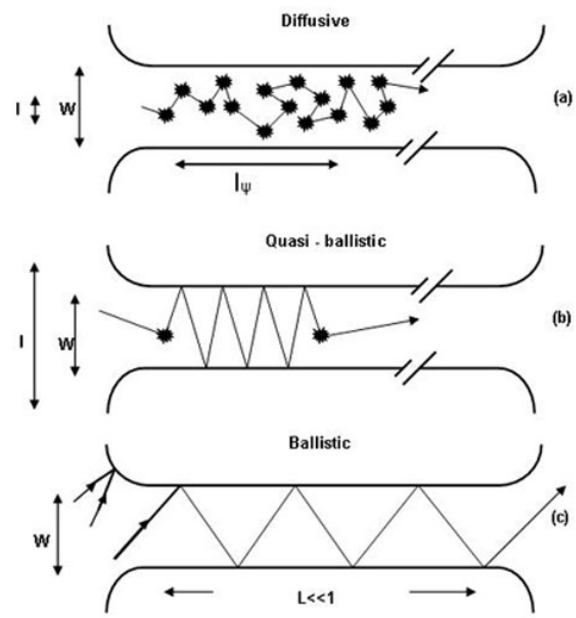
Referee #1 and #2:

- The proposed algorithm is not clear.

Response: In light of the reviewer's recommendation, we now present the algorithm in one-dimensional condition for better understanding and ballistic concept.

- **The ballistic concept is not introduced at all in section 4. Referee #1**

  Response: The **ballistic** concept is taken from Condensed Matter physics.(please see the introduction in this link http://asdn.net/asdn/electronics/transport.php).
  For Electron Transport in Semiconductors. There are three types of transportation behaviour: Diffusive, quasi- Ballistic and Ballistic. Please see the attached figure. The 'Ballistic' means transportation is exponentially accelerated.



- **The proposed algorithm.**
  Response: Here we demonstrate the algorithm in one-dimensional case, this algorithm is also called quantum walk, for one-dimensional case, please see here: Section

  Discrete Time Quantum Walks https://en.wikipedia.org/wiki/Quantum_walk
  There are two operators, a "coin flip" operator and a conditional shift operator, which are applied repeatedly.
  1. First, the distribution on one-dimensional line (9 nodes: $x = -4\ to\ 4$) is:

$$\{0,0,0,0,1,0,0,0,0\}$$

The state on the middle node (x=0) is $\frac{1}{\sqrt{2}}\ (|left\rangle + i\ |right\rangle)$. The left state means go left and the right state means go right, the state is in the coin Hilbert space. $|left\rangle$ corresponds to $\binom{1}{0}$ and $|left\rangle$ corresponds to $\binom{0}{1}$.

2. ***(Coin space operation)*** Then we apply the coin operator, in one-dimensional case the coin operator is the Hadamard Gate. $H = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}$, apply coin operator on the state

   $H\frac{1}{\sqrt{2}}\ (|left\rangle + i\ |right\rangle) = \frac{1}{\sqrt{2}}\ H\binom{1}{i} = \frac{1}{2}\ \binom{1+i}{1-i} = \frac{1}{2}\ ((1+i)|left\rangle + \frac{1}{2}\ (1-i)|right\rangle$

   (Spatial space operation) Now the line is $\{0,0,0,0,1,0,0,0,0\}$with a state $\frac{1}{2}\ (1+i)|left\rangle + \frac{1}{2}\ (1-i)|right\rangle$ on $x = 0$. For every node, move the $|left\rangle$ state amplitude to left node and $|right\rangle$ to right node.

   Now the line is $\{0,0,0,\frac{1}{2}\ (1+i), 0, \frac{1}{2}\ (1-i), 0,0,0\}$, with pure state $|left\rangle$ on $x = -1$ and pure state $|right\rangle$ on $x = 1$.

   The probability is the norm (multiply the conjugate complex number) of the state amplitude: the distribution on a line becomes:

   $$\{0,0,0,\frac{1}{2}\ 0, \frac{1}{2}, 0,0,0\}$$

   with pure state $|left\rangle$ on $x = -1$ and pure state $|right\rangle$ on $x = 1$.

3. ***Coin space operation:*** the amplitude distribution on a line last moment: $\{0,0,0,\frac{1}{2}\ (1+i), 0, \frac{1}{2}\ (1-i), 0,0,0\}$

   Using coin operator :$H\frac{(1+i)}{2}\binom{1}{0} = \frac{1+i}{2\sqrt{2}}\binom{1}{1}$ on $x = -1$ and $H\frac{(1-i)}{2}\binom{0}{1} = \frac{1-i}{2\sqrt{2}}\binom{1}{-1}$. For $x = -1$, $\frac{1+i}{2\sqrt{2}}\binom{1}{1} = \frac{1+i}{2\sqrt{2}}|left\rangle + \frac{1+i}{2\sqrt{2}}|right\rangle$, moves the $|left\rangle$ state amplitude to left node and $|right\rangle$ to right node. Same as For $x = 1$.

   (Spatial space operation) the amplitude on the line becomes

   $$\{0,0,\frac{1+i}{2\sqrt{2}}|left\rangle, 0, \frac{1+i}{2\sqrt{2}}|left\rangle + \frac{1-i}{2\sqrt{2}}|right\rangle, 0, \frac{1-i}{2\sqrt{2}}|right\rangle, 0,0,0\} =$$

   $$\{0,0,\frac{1+i}{2\sqrt{2}}, 0, \frac{1}{\sqrt{2}}, 0, \frac{1-i}{2\sqrt{2}}, 0,0,0\}$$

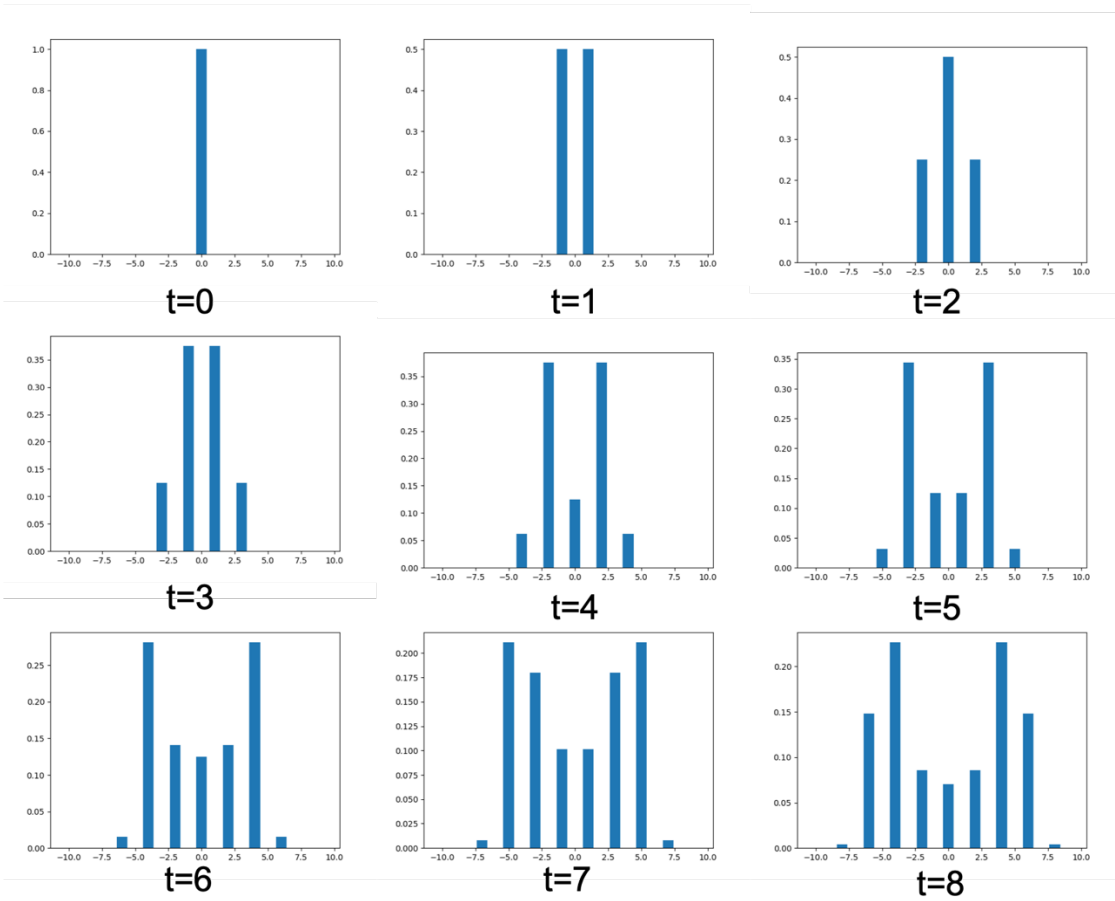
   With $|left\rangle$ at $x = -2$, $\frac{1}{2}\big((1+i)|left\rangle + (1-i)|right\rangle\big)$ at $x = 0$ and $|right\rangle\ at\ x = 2$.

   The probability is the norm (multiply the conjugate complex number)

   $$\{0,0,\frac{1}{4}, 0, \frac{1}{2}, 0, \frac{1}{4}, 0,0\}$$

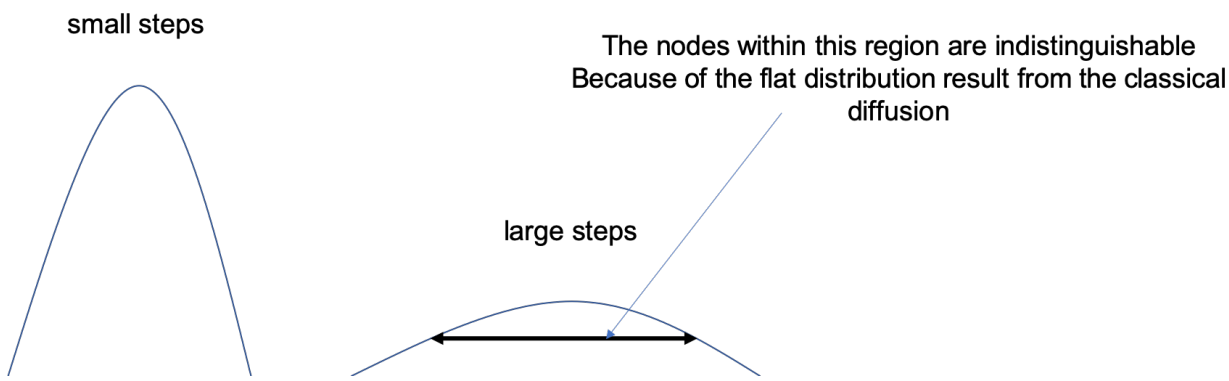
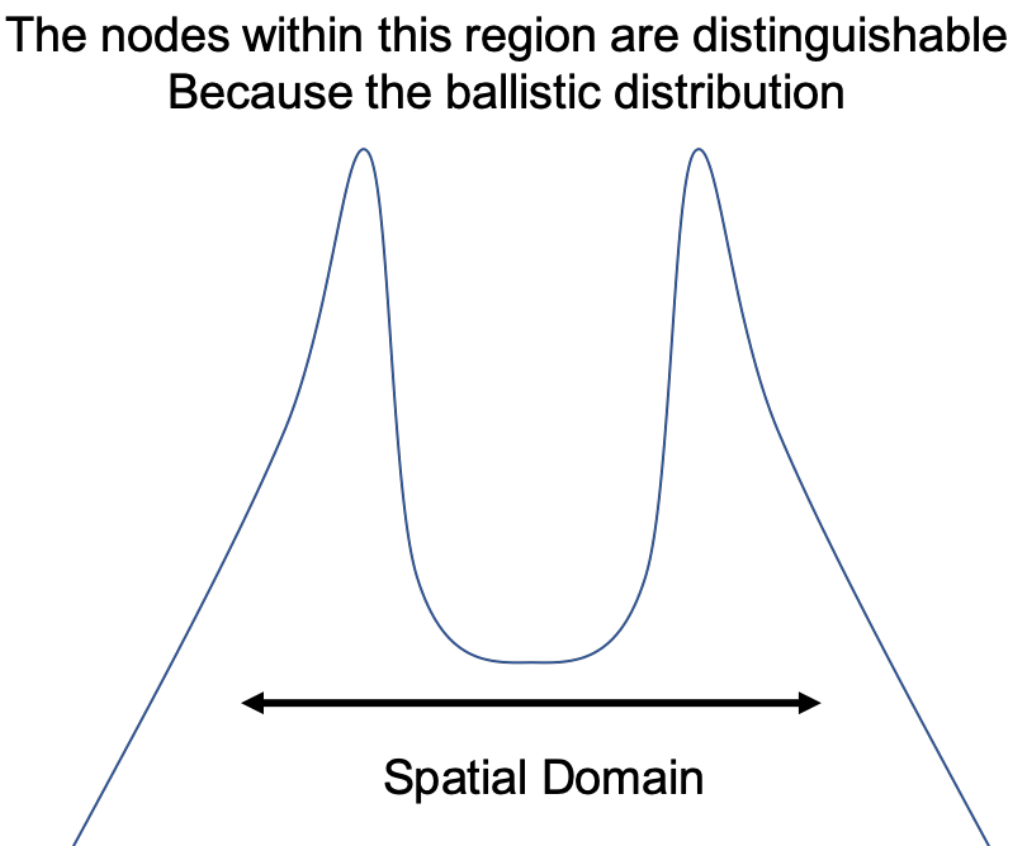
   Repeat the two operation again and again.

   Here we plot ***Probability*** (not amplitude) evolution on a line with 21 nodes.



<u>Referee #3 the over smooth problem:</u>

The smooth problem means after apply traditional Laplacian-based matrix on a manifold; the distribution will become more and more **'flat'** on the spatial domain, as shown in the figure below:



But the ballistic diffusion avoids this problem, see the attached figure: