

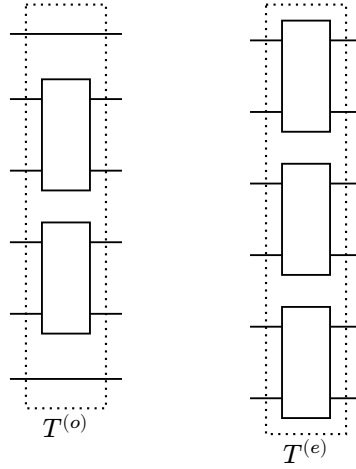
Calculate α

2024-04-17

Bian Kaiming

1. The tensor and the vector space

Let $T^{(o)}$ be the odd layer of T gates, and $T^{(e)}$ be the even layer of T gates. Then we have the following circuits:



Now, alternately apply the odd and even layers of T gates to the $|\gamma_1 \gamma_{2n}\rangle$

$$T^{(\text{whole})}(b_1, t) = T^{(o)b_2} \left(\prod_{i=0}^{t-b_2} T^{(e)} T^{(o)} \right) T^{(e)b_1},$$

where $b_1, b_2 \in \{0, 1\}$, $t + b_1$ stands for the number of layers. The output states must in the vector space spanned by the following basis

$$\begin{aligned} &|Z_i\rangle, \quad \left| X_i \left(\prod_{k=i+1}^{j-1} Z_k \right) X_j \right\rangle, \quad \left| X_i \left(\prod_{k=i+1}^{j-1} Z_k \right) Y_j \right\rangle, \\ &\left| Y_i \left(\prod_{k=i+1}^{j-1} Z_k \right) X_j \right\rangle, \quad \left| Y_i \left(\prod_{k=i+1}^{j-1} Z_k \right) Y_j \right\rangle \end{aligned}$$

Let $M_i = \frac{1}{\sqrt{2}}(X_i + Y_i)$, the space

$$V := \text{span} \left\{ |Z_i\rangle, \left| M_i \left(\prod Z_k \right) M_j \right\rangle \right\}$$

is the image subspace for all $T^{(\text{whole})}(b_1, t)$ with $b_1 + t > 0$ if the input state is limit to Γ_2 . Thus, the action of $T^{(\text{whole})}(b_1, t)$ could always be written in the following form

$$T^{(\text{whole})}(b_1, t)|\gamma_1 \gamma_{2n}\rangle\rangle = \sum P(i, i, t)|Z_i\rangle\rangle + \sum_{i < j} P(i, j, t)|M_i(\prod Z_k)M_j\rangle\rangle.$$

The action of the tensor could be simplified by studying the coefficients $P(i, j, t)$.

2. Propagation in polynomials space

To simplify the discussion, we start with a special case: $b_1 = 1, b_2 = 0$, and the number of wires is an even number $2N$. In this case, the whole tensor $T^{(\text{whole})}$ could be written as

$$T^{(\text{whole})}(1, t) = (T^{(e)}T^{(o)})^t T^{(e)}.$$

Then, we lift the V into the space of the second order $2N$ -dimensional polynomials

$$W := \text{span}\left\{\sum_{i,j=1}^{2N} c_{i,j} x_i x_j\right\}$$

We can prove that the space V is isometric to the space W by ϕ ,

$$\begin{aligned}\phi : V &\rightarrow W \\ |M_i(\prod Z_k)M_j\rangle\rangle &\rightarrow x_i x_j \\ |Z_i\rangle\rangle &\rightarrow x_i^2.\end{aligned}$$

Let $T_p^{(2N)}(t)$ be the map $\phi T^{(\text{whole})}(1, t)\phi^{-1}$, the following diagram commutes.

$$\begin{array}{ccc} V & \xrightarrow{T^{(\text{whole})}(1, t)} & V \\ \uparrow \phi & & \uparrow \phi \\ W & \xrightarrow{T_p^{(2N)}(t)} & W \end{array}$$

Now, let's consider the action of the tensor $T_p^{(2N)}(t)$ on the space W . Similarly, we could write down the recursive relation of coefficients $a_{i,j}$.

When $t = 0$, the transforming state $T^{(e)}|\gamma_1 \gamma_{4N}\rangle\rangle$ to W , and we got $\frac{1}{4}(x_1 x_{2N} + x_1 x_{2N-1} + x_2 x_{2N} + x_2 x_{2N-1})$. Suppose at t , the vector in W is $\sum c_i(t) c'_j(t) x_i x_j$,

$$\begin{aligned}
& T_p^{(2N)}(t+1) \left(\frac{1}{4} (x_1 x_{2N} + x_1 x_{2N-1} + x_2 x_{2N} + x_1 x_{2N-1}) \right) \\
&= T^{(e)} T^{(o)} T_p^{(2N)}(t) \left(\frac{1}{4} (x_1 x_{2N} + x_1 x_{2N-1} + x_2 x_{2N} + x_1 x_{2N-1}) \right) \\
&= T^{(e)} T^{(o)} \sum c_i(t) c'_j(t) x_i x_j
\end{aligned}$$

Then, the action of $\phi T^{(e)} T^{(o)} \phi^{-1}$ on this vector is

$c_i c'_j x_i x_j$	$\phi T^{(e)} T^{(o)} \phi^{-1} (c_i c'_j x_i x_j)$
$i = j = 1$	$\frac{1}{6} (c_1 x_1 + c_1 x_2) (c'_2 x_1 + c'_2 x_2)$
$i = 1, j = 2, 3$	$\frac{1}{8} (c_1 x_1 + c_1 x_2) \left(\frac{4}{3} c'_2 x_1 + \frac{4}{3} c'_2 x_2 + c'_2 x_3 + c'_2 x_4 \right)$
$i = 1, j > 3$	$\frac{1}{8} (c_1 x_1 + c_1 x_2) \left(c'_j x_{j-2+\eta_j} + c'_j x_{j-1+\eta_j} + c'_j x_{j+\eta_j} + c'_j x_{j+1+\eta_j} \right)$
$1 < i < 2N,$ $i = j$	$\frac{1}{24} (c_i x_{i-2+\eta_i} + c_i x_{i-1+\eta_i} + c_i x_{i+\eta_i} + c_i x_{i+1+\eta_i})$ $(c'_j x_{j-2+\eta_j} + c'_j x_{j-1+\eta_j} + c'_j x_{j+\eta_j} + c'_j x_{j+1+\eta_j})$ $-\frac{1}{72} (c_i x_{i-2+\eta_i} + c_i x_{i-1+\eta_i}) (c'_j x_{j-2+\eta_j} + c'_j x_{j-1+\eta_j})$ $-\frac{1}{72} (c_i x_{i+\eta_i} + c_i x_{i+1+\eta_i}) (c'_j x_{j+\eta_j} + c'_j x_{j+1+\eta_j})$
$1 < i < 2N,$ i is even, $j = i + 1$	$\frac{1}{12} c_i c_{j'} (c_i x_{i-2+\eta_i} + c_i x_{i-1+\eta_i} + c_i x_{i+\eta_i} + c_i x_{i+1+\eta_i})^2$ $-\frac{1}{36} (c_i x_{i-2+\eta_i} + c_i x_{i-1+\eta_i}) (c'_j x_{j-2+\eta_j} + c'_j x_{j-1+\eta_j})$ $-\frac{1}{36} (c_i x_{i+\eta_i} + c_i x_{i+1+\eta_i}) (c'_j x_{j+\eta_j} + c'_j x_{j+1+\eta_j})$
$1 < i < 2N,$ $i + \eta_i \leq j \leq i + \eta_i + 2$	$\frac{1}{16} (c_i x_{i-2+\eta_i} + c_i x_{i-1+\eta_i} + c_i x_{i+\eta_i} + c_i x_{i+1+\eta_i})$ $(c'_j x_{j-2+\eta_j} + c'_j x_{j-1+\eta_j} + c'_j x_{j+\eta_j} + c'_j x_{j+1+\eta_j})$ $+\frac{1}{48} (c_i x_{i+\eta_i} + c_i x_{i+1+\eta_i}) (c'_j x_{j-2+\eta_j} + c'_j x_{j-1+\eta_j})$
$1 < i < 2N,$ $j > i + \eta_i + 2$	$\frac{1}{16} (c_i x_{i-2+\eta_i} + c_i x_{i-1+\eta_i} + c_i x_{i+\eta_i} + c_i x_{i+1+\eta_i})$ $(c'_j x_{j-2+\eta_j} + c'_j x_{j-1+\eta_j} + c'_j x_{j+\eta_j} + c'_j x_{j+1+\eta_j})$

$c_i c'_j x_i x_j$	$\phi T^{(e)} T^{(o)} \phi^{-1} (c_i c'_j x_i x_j)$
$i = j = 2N$	$\frac{1}{6} (c_{2N} x_{2N-1} + c_{2N} x_{2N}) (c'_{2N} x_{2N-1} + c'_{2N} x_{2N})$

Table 1: The action of the tensor $\phi T^{(e)} T^{(o)} \phi^{-1}$ on the space of second order $2N$ -dimensional polynomials.

The subscript η_i is defined as $\eta_i := 1 - (i \bmod 2)$. We can see that, c_{2i-1} and c_{2i} are always the same. So do c'_{2j-1} and c'_{2j} . Let $b_i = 2c_{2i-1} = 2c_{2i}$ and $b'_j = 2c'_{2j-1} = 2c'_{2j}$, we could further simplify the action of the tensor in the space of second order N -dimensional polynomials W_N . For simplicity, we define a “free” recursive relation in W_N

$$P(i, t+1) = \begin{cases} \frac{1}{4} (P(i-1, t) + 2P(i, t) + P(i+1, t)) , & i \neq 1 \text{ or } N \\ \frac{1}{4} (P(i-1, t) + 2P(i, t) + P(i+1, t)) , & i = 1 \text{ or } N \end{cases} . \quad (1)$$

We call it “free” because $b_i(t)b'_j(t) = P(i, t)P(j, t)$ if i and j are not “collide” with each other (which means $|i - j| > 3$). And the solution of Eq. (1) is a propagating wave. Refs. [1] provide the solution of this equation,

$$P_{n_0}(n, t) = \frac{1}{N} + \frac{2}{N} \sum_{k=1}^{N-1} \cos\left(\left(n - \frac{1}{2}\right) \frac{\pi k}{N}\right) \cos\left(\left(n_0 - \frac{1}{2}\right) \frac{\pi k}{N}\right) \cos^{2t} \frac{\pi k}{2N}, \quad (2)$$

where n_0 is the initial state. The term $P_{n_0}(n, t)$ also called the propagator.

For our case, there are 2 propagators, which are P_1 and P_N . And the initial state is $x_1 x_N$. Let $\phi()$

Now, let's plug $b_i = 2c_{2i-1} = 2c_{2i}$ and $b'_j = 2c'_{2j-1} = 2c'_{2j}$ into Table 1. More concretely, let ϕ' be the map

$$\begin{aligned} \phi' : W_N &\rightarrow W_{2N} \\ y_i y_j &\rightarrow \frac{1}{4} (x_{2i-1} + x_{2i}) (x_{2j-1} + x_{2j}). \end{aligned}$$

If we consider the subspace W'_{2N} of W_{2N} , where $W'_{2N} := \text{span}((x_{2i-1} + x_{2i})(x_{2j-1} + x_{2j}))$ (it means $c_{2i-1} = c_{2i}$ and $c'_{2j-1} = c'_{2j}$), the ϕ' will be the isometric between W_N and W'_{2N} . Thus, the following diagram commutes.

$$\begin{array}{ccc}
V & \xrightarrow{T^{(\text{whole})}(1, t)} & V \\
\updownarrow \phi & & \updownarrow \phi \\
W'_{2N} & \xrightarrow{T_p^{(2N)}(t)} & W'_{2N} \\
\updownarrow \phi' & & \updownarrow \phi' \\
W_N & \xrightarrow{T_p^{(N)}(t)} & W_N
\end{array}$$

For simpliness, let

$$F(y_i) = \begin{cases} \frac{3}{4}y_1 + \frac{1}{4}y_2, & i = 1 \\ \frac{1}{4}y_{i-1} + \frac{1}{2}y_i + \frac{1}{4}y_{i+1}, & 1 < i < N \\ \frac{3}{4}y_N + \frac{1}{4}y_{N-1}, & i = N \end{cases}$$

Then we get

$y_i y_j$	$T^{(e)}T^{(o)}$
$i = j = 1$	$F(y_1)F(y_1) - \frac{5}{144}(y_1 + y_2)^2 + \frac{1}{36}y_1 y_2$
$i = 1, j = 2$	$F(y_1)F(y_2) + \left(\frac{5}{144}\right)(y_1^2) + \left(\frac{1}{24}\right)y_1 y_2 + \left(\frac{1}{72}\right)(y_2^2)$
$i = 1, j = 3$	$F(y_1)F(y_3) + \frac{1}{48}y_2^2$
$1 < i < N, j = i$	$F(y_i)F(y_i) - \frac{5}{144}y_{i-1}^2 - \frac{5}{48}y_{i-1}y_i - \frac{1}{16}y_{i-1}y_{i+1}$ $-\frac{1}{9}y_i^2 - \frac{5}{48}y_i y_{i+1} - \frac{5}{144}y_{i+1}^2$
$1 < i < N, j = i + 1$	$F(y_i)F(y_{i+1}) + \frac{1}{72}y_i^2 + \frac{1}{24}y_i y_{i+1} + \frac{1}{72}y_{i+1}^2$
$1 < i < N, j = i + 2$	$F(y_i)F(y_{i+2}) + \frac{1}{48}y_{i+1}^2$

$y_i y_j$	$T^{(e)} T^{(o)}$
$i = j = N$	$F(y_N)F(y_N) - \frac{5}{144}(y_N + y_{N-1})^2 + \frac{1}{36}y_{N-1}y_N$
other cases when $i \leq j$	$F(y_i)F(y_j)$

Table 2: The action of the tensor $T^{(e)}T^{(o)}$ on the space of second order N-dimensional polynomials.

这个 table 的计算实在是太太太太折磨人了。详细计算我放在了 Section 4 中。

3. The interaction term

let $b(i, j, t) = P_1(i, t)P_N(j, t) + I(i, j, t)$. Then,

$$|\psi(t)\rangle = \sum_{i,j} P_1(i, t)P_N(j, t)y_i y_j - \sum_{i,j} I(i, j, t)y_i y_j. \quad (3)$$

From simpleness, let the terms in Table 2 be $F(y_i)F(y_j) + R(i, j)$. Then we get

$$\begin{aligned} |\psi(t+1)\rangle &= \sum_{i,j} P_1(i, t)P_N(j, t)(F(y_i)F(y_j) + R(i, j)) - \sum_{i,j} I(i, j, t)(F(y_i)F(y_j) + R(i, j)) \\ &= \sum_{i,j} P_1(i, t+1)P_N(j, t+1)y_i y_j + \sum_{i,j} P_1(i, t)P_N(i, t)R(i, j) \\ &\quad - \sum_{i,j} I(i, j, t)(F(y_i)F(y_j) + R(i, j)) \end{aligned}$$

这里又又又为了简洁性, 定义

$$\begin{aligned} F_f^{(1)} : \text{Func}(i, j, t) &\mapsto \begin{cases} \frac{1}{4} \text{Func}(i-1, j, t) + \dots & \text{if } i > 1 \\ \frac{3}{4} \text{Func}(i, j, t) + \dots & \text{if } i = 1 \end{cases} \\ F_f^{(2)} : \text{Func}(i, j, t) &\mapsto \begin{cases} \frac{1}{4} \text{Func}(i, j-1, t) + \dots & \text{if } j > 1 \\ \frac{3}{4} \text{Func}(i, j, t) + \dots & \text{if } j = 1 \end{cases} \end{aligned}$$

By using Eq. (3) to expand $|\psi(t+1)\rangle$, we have

$$\begin{aligned}
& I(i, j, t+1) \\
&= -\frac{\partial}{\partial y_i} \frac{\partial}{\partial y_j} \left(\sum_{i,j} P_1(i, t) P_N(i, t) R(i, j) - \sum_{i,j} I(i, j, t) (F(y_i) F(y_j) + R(i, j)) \right) \quad (4) \\
&= F_f^{(1)}(I)(i, j, t) F_f^{(2)}(I)(i, j, t) - \sum_{l,k} \frac{\partial}{\partial y_i} \frac{\partial}{\partial y_j} \left((P_1(l, t) P_N(k, t) - I(l, k, t)) R(l, k) \right)
\end{aligned}$$

可以从表中看见，仅当 $l \in \{i-1, i, i+1\} \cap \mathbb{Z}_+$, $k \in \{j-1, j, j+1\} \cap \mathbb{Z}_+$, $|l-k| \leq 2$ 时，Eq. (4) 中的第二项才不为 0。同时，我们知道，若其不为 0，则有

$$-\frac{1}{9} \leq \frac{\partial}{\partial y_i} \frac{\partial}{\partial y_j} R(l, k) \leq \frac{1}{24}.$$

由它们的系数 $b(i, j, t) > 0$ ，我们可以知道 $P_1(l, t) P_N(k, t) > I(l, k, t)$ 对所有时刻 t 恒成立。

由于初始状态下， $I(i, j, t) = 0 \forall i, j$ 。

现在我们来了解一下第二项会是什么。这里主要就是看 R 是什么。这时候我们又开始快乐打表了。打表的一些细节仍然放在 Section 4 中。为了简单，在下面表格中用 D_{ij} 指代 $P_1(i, t) P_{j(i, t)}$ 或 $I(i, j, t)$ 。这里需要注意的是， $y_i y_i$ 产生的 $y_i y_{i+1}$ 会写成 $y_i y_{i+1} + y_{i+1} y_i$ 。因此，在生成下述表格时， $j = i+1$ 那一栏中，在从 Table 2 中写出 D_{ii} 的系数时需要除一个 2。

$D(i, j, t+1)$	$\sum \frac{\partial^2}{\partial y_i \partial y_j} D_{lk} R(l, k)$
$i = j = 1$	$\frac{5}{144}(-D_{11} - D_{22} + D_{12} + D_{21})$
$i = 1, j = 2$	$-\frac{1}{48}D_{11} + \frac{1}{24}D_{12} - \frac{5}{96}D_{22}$
$1 < i = j < N$	$\begin{pmatrix} -\frac{5}{144} & \frac{1}{72} & \frac{1}{48} \\ \frac{1}{72} & -\frac{1}{9} & \frac{1}{72} \\ \frac{1}{48} & \frac{1}{72} & -\frac{5}{144} \end{pmatrix}$
$1 < i < N, j = i+1$	$-\frac{5}{96}D_{ii} + \frac{1}{24}D_{i, i+1} - \frac{5}{96}D_{i+1, i+1}$

$D(i, j, t + 1)$	$\sum \frac{\partial^2}{\partial y_i \partial y_j} D_{lk} R(l, k)$
$i = N$	$\frac{5}{144}(-D_{N,N} - D_{N-1,N-1} + D_{N,N-1} + D_{N-1,N})$

Table 3: The action of the operator $\frac{\partial^2}{\partial y_i \partial y_j}$ on the terms in Table 2.

令 $I_{i,j} = I(i, j, t + 1) = I(i, j, t)$, 则由 (4)

$$I_{i,j} = F_f^{(1)}(I)(i, j, t) F_f^{(2)}(I)(i, j, t) - \sum_{l,k} \frac{\partial}{\partial y_i} \frac{\partial}{\partial y_j} \left((P_1(l, t) P_N(k, t) - I(l, k, t)) R(l, k) \right)$$

再进行一个均匀的线性组合, 有

$$\begin{aligned} 0 &= \frac{1}{N^2} \sum_{i,j} \left(I_{i,j} - F_f^{(1)}(I)(i, j, t) F_f^{(2)}(I)(i, j, t) \right) \\ &= -\frac{1}{N^2} \sum_{i,j} \sum_{l,k} \frac{\partial}{\partial y_i} \frac{\partial}{\partial y_j} \left((P_1(l, t) P_N(k, t) - I(l, k, t)) R(l, k) \right) \end{aligned}$$

通过查表 Table 3, 和一些代数游戏, 可以得到

$$\begin{aligned} &\frac{1}{48} \sum_{i=1}^{N-2} P_1(i, t) P_N(i+2, t) + \frac{1}{48} \sum_{i=3}^N P_1(i, t) P_N(i-2, t) \\ &+ \frac{5}{72} \sum_{i=1}^{N-1} P_1(i, t) P_N(i+1, t) + \frac{5}{72} \sum_{i=2}^N P_1(i, t) P_N(i-1, t) \\ &- \frac{7}{18} \sum_{i=2}^{N-1} P_1(i, t) P_N(i, t) - \frac{1}{9} P_1(1, t) P_N(1, t) - \frac{1}{9} P_1(N, t) P_N(N, t) \end{aligned}$$

i, j	$\sum \frac{\partial^2}{\partial y_i \partial y_j} D_{lk} R(l, k)$
$i = j = 1$	$\frac{5}{144}(-D_{11} - D_{22} + D_{12} + D_{21})$
$i = 1, j = 2$	$-\frac{1}{24}D_{11} + \frac{1}{24}D_{12} - \frac{5}{48}D_{22}$
$1 < i = j < N$	$\begin{pmatrix} -\frac{5}{144} & \frac{1}{72} & \frac{1}{48} \\ \frac{1}{72} & -\frac{1}{9} & \frac{1}{72} \\ \frac{1}{48} & \frac{1}{72} & -\frac{5}{144} \end{pmatrix}$

i, j	$\sum \frac{\partial^2}{\partial y_i \partial y_j} D_{lk} R(l, k)$
$1 < i < N, j = i + 1$	$-\frac{5}{48}D_{ii} + \frac{1}{24}D_{i,i+1} - \frac{5}{48}D_{i+1,i+1}$
$i = N$	$\frac{5}{144}(-D_{N,N} - D_{N-1,N-1} + D_{N,N-1} + D_{N-1,N})$

4. Proofs

Proof of Table 2: 现在我们想要计算 $T_p^{(N)}(t)$ 在 W_N 中的作用。因此我们需要计算

$$\begin{aligned}
& \phi' \phi T^{(e)} T^{(o)} \phi^{-1} \phi'^{-1} (y_i y_j) \\
&= \phi T^{(e)} T^{(o)} \phi^{-1} \left(\frac{1}{4} (x_{2i-1} + x_{2i}) (x_{2j-1} + x_{2j}) \right) \\
&= \phi T^{(e)} T^{(o)} \phi^{-1} \left(\frac{1}{4} (x_{2i-1} x_{2j-1} + x_{2i-1} x_{2j} + x_{2i} x_{2j-1} + x_{2i} x_{2j}) \right)
\end{aligned}$$

相当于对于每一个 $x_{2i-1} x_{2j-1}$ 这样的项进行查表。我们现在来分析不同的 y 的映射。为了简化符号, 这里记 $S_N = \phi' \phi T^{(e)} T^{(o)} \phi^{-1} \phi'^{-1}$, $S_{2N} = \phi T^{(e)} T^{(o)} \phi^{-1}$.

$$\begin{aligned}
\phi' (y_1 y_1) &= \frac{1}{4} (x_1 x_1 + 2x_1 x_2 + x_2 x_2) \\
S_N (y_1 y_1) &= \frac{1}{4} (S_{2N}(x_1 x_1) + S_{2N}(2x_1 x_2) + S_{2N}(x_2 x_2))
\end{aligned}$$

依据 Table 1, 我们有

$$\begin{aligned}
S_N(y_1 y_1) &= \frac{1}{4} \left(\right. \\
&\quad \frac{1}{6} (x_1 + x_2)(x_1 + x_2) + \\
&\quad \left(\frac{1}{4} \right) \left(\left(\frac{4}{3} \right) x_1 + \left(\frac{4}{3} \right) x_2 + x_3 + x_4 \right) (x_1 + x_2) + \\
&\quad - \left(\frac{1}{72} \right) ((x_1 + x_2)^2) + \left(\frac{1}{24} \right) ((x_1 + x_2 + x_3 + x_4)^2) - \left(\frac{1}{72} \right) ((x_3 + x_4)^2) \\
&\quad \left. \right) \\
&= \left(\frac{19}{144} \right) (x_1^2) + \left(\frac{19}{72} \right) x_1 x_2 + \left(\frac{1}{12} \right) x_1 x_3 + \left(\frac{1}{12} \right) x_1 x_4 \\
&\quad + \left(\frac{19}{144} \right) (x_2^2) + \left(\frac{1}{12} \right) x_2 x_3 + \left(\frac{1}{12} \right) x_2 x_4 \\
&\quad + \left(\frac{1}{144} \right) (x_3^2) + \left(\frac{1}{72} \right) x_3 x_4 + \left(\frac{1}{144} \right) (x_4^2)
\end{aligned}$$

我们想要和“自由演化”进行对比。而 $y_1 y_1$ 自由演化的结果是

$$\begin{aligned}
F(y_1 y_1) &= \frac{1}{16} (3y_1 + y_2)(3y_1 + y_2) \\
&= \frac{1}{16} \left(\frac{3}{2} x_1 + \frac{3}{2} x_2 + \frac{1}{2} x_3 + \frac{1}{2} x_4 \right) \left(\frac{3}{2} x_1 + \frac{3}{2} x_2 + \frac{1}{2} x_3 + \frac{1}{2} x_4 \right) \\
&= \left(\frac{9}{64} \right) (x_1^2) + \left(\frac{9}{32} \right) x_1 x_2 + \left(\frac{3}{32} \right) x_1 x_3 + \left(\frac{3}{32} \right) x_1 x_4 \\
&\quad + \left(\frac{9}{64} \right) (x_2^2) + \left(\frac{3}{32} \right) x_2 x_3 + \left(\frac{3}{32} \right) x_2 x_4 + \left(\frac{1}{64} \right) (x_3^2) \\
&\quad + \left(\frac{1}{32} \right) x_3 x_4 + \left(\frac{1}{64} \right) (x_4^2)
\end{aligned}$$

二者之差为

$$\begin{aligned}
S_N(y_1 y_1) - F(y_1 y_1) &= -\left(\frac{5}{576}\right)(x_1^2) - \left(\frac{5}{288}\right)x_1 x_2 - \left(\frac{1}{96}\right)x_1 x_3 - \left(\frac{1}{96}\right)x_1 x_4 \\
&\quad - \left(\frac{5}{576}\right)(x_2^2) - \left(\frac{1}{96}\right)x_2 x_3 - \left(\frac{1}{96}\right)x_2 x_4 \\
&\quad - \left(\frac{5}{576}\right)(x_3^2) - \left(\frac{5}{288}\right)x_3 x_4 - \left(\frac{5}{576}\right)(x_4^2) \\
&= -\frac{5}{576}(x_1 + x_2 + x_3 + x_4)^2 + \frac{1}{144}(x_1 + x_2)(x_3 + x_4) \\
&= -\frac{5}{144}(y_1 + y_2)^2 + \frac{1}{36}y_1 y_2
\end{aligned}$$

接下来, 算 $S_N(y_1 y_2)$

$$\begin{aligned}
S_N(y_1 y_2) &= \frac{1}{4}(S_{2N}(x_1 x_3) + S_{2N}(x_1 x_4) + S_{2N}(x_2 x_3) + S_{2N}(x_2 x_4)) \\
&= \frac{1}{4}\left(\frac{1}{8}\left(\frac{4}{3}x_1 + \frac{4}{3}x_2 + x_3 + x_4\right)(x_1 + x_2) \right. \\
&\quad \left. + \frac{1}{8}(x_3 + x_4 + x_5 + x_6)(x_1 + x_2) \right. \\
&\quad \left. - \left(\frac{1}{36}\right)((x_1 + x_2)^2) + \left(\frac{1}{12}\right)((x_1 + x_2 + x_3 + x_4)^2) - \left(\frac{1}{36}\right)((x_3 + x_4)^2) \right. \\
&\quad \left. + \frac{1}{16}(x_1 + x_2 + x_3 + x_4)(x_3 + x_4 + x_5 + x_6) + \frac{1}{48}(x_3 + x_4)^2 \right. \\
&\quad \left. \right) = \left(\frac{2}{9}\right)(y_1^2) + \left(\frac{23}{48}\right)y_1 y_2 + \left(\frac{3}{16}\right)y_1 y_3 + \left(\frac{5}{36}\right)(y_2^2) + \left(\frac{1}{16}\right)y_2 y_3
\end{aligned}$$

$$F(y_1)F(y_2) = \left(\frac{3}{4}y_1 + \frac{1}{4}y_2\right)\left(\frac{1}{4}y_1 + \frac{1}{2}y_2 + \frac{1}{4}y_3\right)$$

$$S_N(y_1 y_2) = F(y_1)F(y_2) + \left(\frac{5}{144}\right)(y_1^2) + \left(\frac{1}{24}\right)y_1 y_2 + \left(\frac{1}{72}\right)(y_2^2)$$

接下来, 算 $S_N(y_1 y_3)$

$$S_N(y_1 y_3) = F(y_1)F(y_3) + \frac{1}{48}y_2^2$$

然后, $j > 3$ 时

$$S_N(y_1 y_j) = F(y_1)F(y_j)$$

然后, $i > 1, i = j$ 时,

$$\begin{aligned}
S_N(y_i y_j) &= \frac{1}{4}(S_N(x_{2i-1}x_{2j-1}) + S_N(x_{2i-1}x_{2j}) + S_N(x_{2i}x_{2j-1}) + S_N(x_{2i}x_{2j})) \\
&= \frac{1}{4}(S_N(x_{2i-1}x_{2i-1}) + 2S_N(x_{2i-1}x_{2i}) + S_N(x_{2i}x_{2i})) \\
&= \frac{1}{4}\left(\frac{1}{24}(x_{2i-3} + x_{2i-2} + x_{2i-1} + x_{2i})^2 \right. \\
&\quad - \frac{1}{72}(x_{2i-3} + x_{2i-2})^2 - \frac{1}{72}(x_{2i-1} + x_{2i})^2 \\
&\quad + \frac{1}{24}(x_{2i-1} + x_{2i} + x_{2i+1} + x_{2i+2})^2 \\
&\quad - \frac{1}{72}(x_{2i-1} + x_{2i})^2 - \frac{1}{72}(x_{2i+1} + x_{2i+2})^2 \\
&\quad + \frac{1}{16}(x_{2i-3} + x_{2i-2} + x_{2i-1} + x_{2i})(x_{2i-1} + x_{2i} + x_{2i+1} + x_{2i+2}) \\
&\quad \left. + \frac{1}{48}(x_{2i-1} + x_{2i})^2 \right) \\
&= \frac{1}{24}(y_{i-1} + y_i)^2 - \frac{1}{72}(y_{i-1})^2 - \frac{1}{72}(y_i)^2 \\
&\quad + \frac{1}{24}(y_i + y_{i+1})^2 - \frac{1}{72}(y_i)^2 - \frac{1}{72}(y_{i+1})^2 \\
&\quad + \frac{1}{16}(y_{i-1} + y_i)(y_i + y_{i+1}) + \frac{1}{48}(y_i)^2 \\
S_N(y_i y_j) &= F(y_i)F(y_j) - \left(\frac{5}{144}\right)(y_{i-1}^2) - \left(\frac{5}{48}\right)y_{i-1}y_i - \left(\frac{1}{16}\right)y_{i-1}y_{i+1} \\
&\quad - \left(\frac{1}{9}\right)(y_i^2) - \left(\frac{5}{48}\right)y_i y_{i+1} - \left(\frac{5}{144}\right)(y_{i+1}^2)
\end{aligned}$$

然后, $i > 1, j = i + 1$ 时,

$$\begin{aligned}
S_N(y_i y_j) &= \frac{1}{4}(S_N(x_{2i-1}x_{2i+1}) + S_N(x_{2i-1}x_{2i+2}) + S_N(x_{2i}x_{2i+1}) + S_N(x_{2i}x_{2i+2})) \\
&= \frac{1}{4} \left(\begin{aligned} &\frac{1}{16}(x_{2i-3} + x_{2i-2} + x_{2i-1} + x_{2i})(x_{2i-1} + x_{2i} + x_{2i+1} + x_{2i+2}) \\ &+ \frac{1}{48}(x_{2i-1} + x_{2i})^2 \\ &+ \frac{1}{16}(x_{2i-3} + x_{2i-2} + x_{2i-1} + x_{2i})(x_{2i+1} + x_{2i+2} + x_{2i+3} + x_{2i+4}) \\ &+ \frac{1}{12}(x_{2i-1} + x_{2i} + x_{2i+1} + x_{2i+2})^2 \\ &- \frac{1}{36}(x_{2i-1} + x_{2i})^2 - \frac{1}{36}(x_{2i+1} + x_{2i+2})^2 \\ &+ \frac{1}{16}(x_{2i-1} + x_{2i} + x_{2i+1} + x_{2i+2})(x_{2i+1} + x_{2i+2} + x_{2i+3} + x_{2i+4}) \\ &+ \frac{1}{48}(x_{2i+1} + x_{2i+2})^2 \end{aligned} \right) \\
&= \frac{1}{16}(y_{i-1} + y_i)(y_i + y_{i+1}) + \frac{1}{48}(y_i)^2 \\
&\quad + \frac{1}{16}(y_i + y_{i+1})(y_{i+1} + y_{i+2}) + \frac{1}{48}(y_{i+1})^2 \\
&\quad + \frac{1}{16}(y_{i-1} + y_i)(y_{i+1} + y_{i+2}) \\
&\quad + \frac{1}{12}(y_i + y_{i+1})^2 - \frac{1}{36}(y_i)^2 - \frac{1}{36}(y_{i+1})^2 \\
S_N(y_i y_j) &= F(y_i)F(y_j) + \left(\frac{1}{72}\right)(y_i^2) + \left(\frac{1}{24}\right)y_i y_{i+1} + \left(\frac{1}{72}\right)(y_{i+1}^2)
\end{aligned}$$

□

Proof of Table 3: 观察 Table 2, 仅有 $y_1 y_1, y_1 y_2, y_2 y_1, y_2 y_2$ 的项可以对 $I(1, 1, t + 1)$ 产生贡献。因此,

$$\begin{aligned}
& \frac{\partial^2}{\partial y_i \partial y_j} P_1(l, t) P_N(k, t) R(l, k) \\
&= \frac{5}{144} (-P_1(1, t) P_N(1, t) - P_1(2, t) P_N(2, t) + P_1(1, t) P_N(2, t) + P_1(2, t) P_N(1, t)) \\
&= -\frac{5}{144} (P_1(1, t) - P_1(2, t)) (P_N(1, t) - P_N(2, t))
\end{aligned}$$

现在重要的就是确认这一项的符号。好在我们是知道 P 的具体形式的。由 Eq. (2) 可以得到

$$\begin{aligned}
P_1(n, t) &= \frac{1}{N} + \frac{2}{N} \sum_{k=1}^{N-1} \cos\left(\left(n - \frac{1}{2}\right) \frac{\pi k}{N}\right) \cos^{2t+1}\left(\frac{\pi k}{2N}\right) \\
P_N(n, t) &= \frac{1}{N} + \frac{2}{N} \sum_{k=1}^{N-1} (-1)^k \cos\left(\left(n - \frac{1}{2}\right) \frac{\pi k}{N}\right) \cos^{2t+1}\left(\frac{\pi k}{2N}\right)
\end{aligned}$$

由 Lemma 4.1 可以得到, $P_1(1, t) - P_1(2, t) < 0$, $P_N(1, t) - P_N(2, t) > 0$ 。因此, $I(1, 1, t+1) > 0$ 。

当 $i = 1, j = 2$ 时

$$\begin{aligned}
& \frac{\partial^2}{\partial y_i \partial y_j} P_1(l, t) P_N(k, t) R(l, k) \\
&= -\frac{1}{144} P_1(1) P_N(1) + \frac{1}{24} P_1(1) P_N(2) \\
&\quad + \frac{1}{24} P_1(2) P_N(1) - \frac{5}{48} P_1(2) P_N(2)
\end{aligned}$$

当 $i = j = 2$ 时

$$\begin{aligned}
& \frac{\partial^2}{\partial y_i \partial y_j} P_1(l, t) P_N(k, t) R(l, k) \\
&= -\frac{5}{144} P_1(1) P_N(1) + \frac{1}{72} P_1(1) P_N(2) + \frac{1}{48} P_1(1) P_N(3) \\
& \quad + \frac{1}{72} P_1(2) P_N(1) - \frac{1}{9} P_1(2) P_N(2) + \frac{1}{72} P_1(2) P_N(3) \\
& \quad + \frac{1}{48} P_1(3) P_N(1) + \frac{1}{72} P_1(3) P_N(2) - \frac{5}{144} P_1(3) P_N(3) \\
&= (P_N(1) \ P_N(2) \ P_N(3)) \begin{pmatrix} -\frac{5}{144} & \frac{1}{72} & \frac{1}{48} \\ \frac{1}{72} & -\frac{1}{9} & \frac{1}{72} \\ \frac{1}{48} & \frac{1}{72} & -\frac{5}{144} \end{pmatrix} \begin{pmatrix} P_1(1) \\ P_1(2) \\ P_1(3) \end{pmatrix}
\end{aligned}$$

可以看到, 当 $1 < i = j < N$ 时 $\frac{\partial^2}{\partial y_i \partial y_j} P_1(l, t) P_N(k, t) R(l, k)$ 都符合上述形式。因此, 我们可以得到

$$\begin{aligned}
& \sum_i \frac{\partial^2}{\partial y_i^2} P_1(l, t) P_N(k, t) R(l, k) \\
&= \sum (P_N(i-1) \ P_N(i) \ P_N(i+1)) \begin{pmatrix} -\frac{5}{144} & \frac{1}{72} & \frac{1}{48} \\ \frac{1}{72} & -\frac{1}{9} & \frac{1}{72} \\ \frac{1}{48} & \frac{1}{72} & -\frac{5}{144} \end{pmatrix} \begin{pmatrix} P_1(i-1) \\ P_1(i) \\ P_1(i+1) \end{pmatrix} \\
&= \sum \text{tr} \left(\begin{pmatrix} -\frac{5}{144} & \frac{1}{72} & \frac{1}{48} \\ \frac{1}{72} & -\frac{1}{9} & \frac{1}{72} \\ \frac{1}{48} & \frac{1}{72} & -\frac{5}{144} \end{pmatrix} \begin{pmatrix} P_1(i-1) \\ P_1(i) \\ P_1(i+1) \end{pmatrix} (P_N(i-1) \ P_N(i) \ P_N(i+1)) \right)
\end{aligned}$$

现在来看看后面这个矩阵

$$\mathcal{M} = \sum \begin{pmatrix} P_1(i-1) \\ P_1(i) \\ P_1(i+1) \end{pmatrix} (P_N(i-1) \ P_N(i) \ P_N(i+1))$$

其矩阵元为

$$\mathcal{M}_{l,m} = \sum_{k=2}^{N-1} P_1(k + \xi_l) P_N(k + \xi_m)$$

其中, $\xi_l = -1, 0, 1$ 。我们知道 $\sum P_1(i, t) = \sum P_N(i, t) = 1$ 。

□

Lemma 4.1: $P_1(i, t)$ 随着 i 单减, $P_N(i, t)$ 随着 i 单增。

Proof:

先将 $P(i, t)$ 从整数域延拓到实数域上。这样就可以对 i 进行求导。此时, 由 Eq.(2) 可以得到

$$\begin{aligned}
P_1(x, t) &= \frac{1}{N} + \frac{2}{N} \sum_{k=1}^{N-1} \cos\left(\left(x - \frac{1}{2}\right) \frac{\pi k}{N}\right) \cos^{2t+1}\left(\frac{\pi k}{2N}\right) \\
\frac{\partial}{\partial x} P_1(x, t) &= -\frac{2\pi}{N} \sum_{k=1}^{N-1} \frac{k}{N} \sin\left(\left(x - \frac{1}{2}\right) \frac{\pi k}{N}\right) \cos^{2t+1}\left(\frac{\pi k}{2N}\right) \\
\frac{\partial}{\partial t} P_1(x, t) &= \frac{2}{N} \sum_{k=1}^{N-1} \cos\left[\frac{k\pi}{2N}\right]^{1+2t} \cos\left[\frac{(-\frac{1}{2}) + i}{N} k\pi\right] \ln\left(\cos^2\left(\frac{k\pi}{2N}\right)\right) \\
P_N(x, t) &= \frac{1}{N} + \frac{2}{N} \sum_{k=1}^{N-1} (-1)^k \cos\left(\left(x - \frac{1}{2}\right) \frac{\pi k}{N}\right) \cos^{2t+1}\left(\frac{\pi k}{2N}\right) \\
\frac{\partial}{\partial x} P_N(x, t) &= -\frac{2\pi}{N} \sum_{k=1}^{N-1} (-1)^k \frac{k}{N} \sin\left(\left(x - \frac{1}{2}\right) \frac{\pi k}{N}\right) \cos^{2t+1}\left(\frac{\pi k}{2N}\right)
\end{aligned}$$

现在关注它们导数的符号。注意到 $\cos\left(\frac{\pi k}{2N}\right)$ 随着 k 增大单减。令 $\kappa = \frac{\pi k}{N} \in (0, \pi)$

$$\begin{aligned}
&\sum k \frac{\pi}{N} \sin\left(\left(x - \frac{1}{2}\right) \frac{\pi k}{N}\right) \cos^{2t+1}\left(\frac{\pi k}{2N}\right) \\
&= \text{Im} \left[\sum \kappa e^{i(x-\frac{1}{2})\kappa} \cos^{2t+1}\left(\frac{\kappa}{2}\right) \right]
\end{aligned}$$

假设 N 趋于无穷, 那么

$$\begin{aligned}
\frac{\partial}{\partial x} P_1(x, t) &\rightarrow -2 \int_0^\pi \kappa \sin\left(\left(x - \frac{1}{2}\right) \kappa\right) \cos^{2t+1}\left(\frac{\kappa}{2}\right) d\kappa \\
P_1(x, t) &= \frac{2}{\pi} \int_0^\pi \cos\left[\left(x - \frac{1}{2}\right) \kappa\right] * \cos\left[\frac{\kappa}{2} * (2t + 1)\right] d\kappa \\
&= \frac{1}{\pi} \left[\frac{\sin[\pi(1+t-x)]}{1+t-x} + \frac{\sin[\pi(t+x)]}{t+x} \right]
\end{aligned}$$

□

$$P(x, t+1) - P(x, t) = -\frac{2}{N} \sum \left(\cos \left[\frac{k\pi}{2N} \right]^{1+2t} \cos \left[\frac{k\pi(-(\frac{1}{2}) + x)}{N} \right] \sin \left[\frac{k\pi}{2N} \right]^2 \right)$$

Lemma 4.2: $I(i, j, i+1)$

Proof:

$$I(i, i, t+1) = F_f^{(1)}(I)(i, j, t) F_f^{(2)}(I)(i, j, t) \\ - \sum_{l,k} \frac{\partial}{\partial y_i} \frac{\partial}{\partial y_j} \left((P_1(l, t) P_N(k, t) - I(l, k, t)) R(l, k) \right)$$

$$\text{令 } \mathcal{M} = \begin{pmatrix} -\frac{5}{144} & \frac{1}{72} & \frac{1}{48} \\ \frac{1}{72} & -\frac{1}{9} & \frac{1}{72} \\ \frac{1}{48} & \frac{1}{72} & -\frac{5}{144} \end{pmatrix}. \text{ 由 Table 3 可以得到}$$

□

Lemma 4.3: $P(x, t+1) - P(x, t)$

Proof:

x	$P(x, t+1) - P(x, t)$
$x = 1$	$\frac{\Gamma[\frac{3}{2} + t]}{\sqrt{\pi}\Gamma[3 + t]}$
$x = 2$	$\frac{(-3 + t)\Gamma[\frac{3}{2} + t]}{\sqrt{\pi}\Gamma[4 + t]}$
$x = 3$	$\frac{(-11 + t)\Gamma[\frac{3}{2} + t]}{\sqrt{\pi}\Gamma[5 + t]}$
$x = 4$	$\frac{(-23 + t)\Gamma[\frac{3}{2} + t]}{\sqrt{\pi}\Gamma[6 + t]}$

从这里可以看出，分母就是简单的 $\Gamma(t + x + 2)$ 。但分子有点诡异

□

Lemma 4.4: $|I(i, j, t)| \leq P_1(i, t)P_N(j, t)$

Proof: 用归纳法证明

当 $t = 1$ 时，成立

假设 $t = n$ 时成立，那么 $t = n + 1$ 时

$$I(t + 1) \geq -P_1(i, t)P_N(j, t) - \sum_{l, k} \frac{\partial}{\partial y_i} \frac{\partial}{\partial y_j} \left((P_1(l, t)P_N(k, t) - I(l, k, t))R(l, k) \right)$$

□

Bibliography

- [1] L. Giuggioli, “Exact spatiotemporal dynamics of confined lattice random walks in arbitrary dimensions: A century after Smoluchowski and Pólya,” *Physical Review X*, vol. 10, no. 2, p. 21045–21046, 2020.