# Generation of true quantum random numbers with on-demand probability distributions via single-photon quantum walks: supplement 

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## 1. DETAILS OF THE THEORETICAL MODEL

Here we present the details of the mathematical expression for our gradient descent (GD) algorithm. The basic idea of our algorithm is iteratively adjusting the splitting ratio of the quantum walk system according to the error between the system output and the target, so that the final single-photon distribution reaches the target distribution. Therefore, the key of our GD-based scheme is deriving the mathematical form of the updated value for the splitting ratio. In the following, we present the mathematical derivation of the updating value in our algorithm.

Without loss of generality, we first consider the splitting ratio at position $m$ in the last walking step of an $n$-step quantum walk system. The schematic of the last walking step is shown in Fig. S1(a). The notation $c_{m, R}^{(n)}\left(c_{m, L}^{n}\right)$ represents the complex amplitude of the coin state $|R\rangle(|L\rangle)$ at the position $m$ in the $n$-th walking step, and $r_{m}^{(n)}$ is the splitting ratio of the $n$-th walking step starting from position $m$. The measured probability and target probability for detecting single photons at position $m$ is denoted by $P_{m}$ and $T_{m}$, respectively. The error $e_{m}$ between $P_{m}$ and $T_{m}$ is defined as $e_{m}=T_{m}-P_{m}$. As we have demonstrated in the main text, the measured probability $P_{m}$ can be written in terms of the complex amplitude of the coin state. Then $P_{m-1}$ and $P_{m+1}$ in Fig. S1(a) can be written as

$$
\begin{align*}
& P_{m-1}=\left|c_{m, L}^{(n)}\right|^{2}+\left|c_{m-2, R}^{(n)}\right|^{2}=\left|a_{m, L}^{(n)}+i \cdot b_{m, L}^{(n)}\right|^{2}+\left|a_{m-2, R}^{(n)}+i \cdot b_{m-2, R}^{(n)}\right|^{2}  \tag{S1}\\
& P_{m+1}=\left|c_{m, R}^{(n)}\right|^{2}+\left|c_{m+2, L}^{(n)}\right|^{2}=\left|a_{m, R}^{(n)}+i \cdot b_{m, R}^{(n)}\right|^{2}+\left|a_{m+2, L}^{(n)}+i \cdot b_{m+2, L}^{(n)}\right|^{2}
\end{align*}
$$

where $a$ and $b$ are the real and imaginary components of $c$, respectively. From Fig. S1(a) we can see that the complex amplitudes $c_{m, L}^{(n)}, c_{m, R}^{(n)}$ can be further expressed in terms of $c_{m-1, R}^{(n-1)}, c_{m+1, L}^{(n-1)}$ and the splitting ratio $r_{m}^{(n)}$ as follows,

$$
\begin{align*}
& c_{m, L}^{(n)}=\sqrt{r_{m}^{(n)}} c_{m+1, L}^{(n-1)}+\sqrt{1-r_{m}^{(n)}} c_{m-1, R}^{(n-1)}  \tag{S2}\\
& c_{m, R}^{(n)}=\sqrt{1-r_{m}^{(n)}} c_{m+1, L}^{(n-1)}-\sqrt{r_{m}^{(n)}} c_{m-1, R}^{(n-1)}
\end{align*}
$$

so the relation between $\left\{a_{m, L}^{(n)}, a_{m, R}^{(n)}\right\}\left(\left\{b_{m, L}^{(n)}, b_{m, R}^{(n)}\right\}\right)$ and $\left\{a_{m-1, R}^{(n-1)}, a_{m+1, L}^{(n)}\right\}\left(\left\{b_{m-1, R}^{(n-1)}, b_{m+1, L}^{(n)}\right\}\right)$ becomes

$$
\begin{align*}
& a_{m, L}^{(n)}=\sqrt{r_{m}^{(n)}} a_{m+1, L}^{(n-1)}+\sqrt{1-r_{m}^{(n)}} a_{m-1, R}^{(n-1)} \\
& a_{m, R}^{(n)}=\sqrt{1-r_{m}^{(n)}} a_{m+1, L}^{(n-1)}-\sqrt{r_{m}^{(n)}} a_{m-1, R}^{(n-1)}  \tag{S3}\\
& b_{m, L}^{(n)}=\sqrt{r_{m}^{(n)}} b_{m+1, L}^{(n-1)}+\sqrt{1-r_{m}^{(n)}} b_{m-1, R}^{(n-1)} \\
& b_{m, R}^{(n)}=\sqrt{1-r_{m}^{(n)}} b_{m+1, L}^{(n-1)}-\sqrt{r_{m}^{(n)}} b_{m-1, R}^{(n-1)}
\end{align*}
$$

By substituting Eq. S3 into Eq. S1, we obtain the mathematical relation between the measured probability and the interested splitting ratio,

$$
\begin{align*}
P_{m-1}= & \left(\sqrt{r_{m}^{(n)}} a_{m+1, L}^{(n-1)}+\sqrt{1-r_{m}^{(n)}} a_{m-1, R}^{(n-1)}\right)^{2}+\left(\sqrt{r_{m}^{(n)}} b_{m+1, L}^{(n-1)}+\sqrt{1-r_{m}^{(n)}} b_{m-1, R}^{(n-1)}\right)^{2} \\
& +\left(\sqrt{1-r_{m-2}^{(n)}} a_{m-1, L}^{(n-1)}-\sqrt{r_{m-2}^{(n)}} a_{m-3, R}^{(n-1)}\right)^{2}+\left(\sqrt{1-r_{m-2}^{(n)}} b_{m-1, L}^{(n-1)}-\sqrt{r_{m-2}^{(n)}} b_{m-3, R}^{(n-1)}\right)^{2} \\
P_{m+1}= & \left(\sqrt{1-r_{m}^{(n)}} a_{m+1, L}^{(n-1)}-\sqrt{r_{m}^{(n)}} a_{m-1, R}^{(n-1)}\right)^{2}+\left(\sqrt{1-r_{m}^{(n)}} b_{m+1, L}^{(n-1)}-\sqrt{r_{m}^{(n)}} b_{m-1, R}^{(n-1)}\right)^{2} \\
& \left.+\left(\sqrt{r_{m+2}^{(n)}} a_{m+3, L}^{(n-1)}+\sqrt{1-r_{m+2}^{(n)}} a_{m+1, R}^{(n-1)}\right)^{2}+\left(\sqrt{r_{m+2}^{(n)}} b_{m+3, L}^{(n-1)}+\sqrt{1-r_{m+2}^{(n)}} b_{m+1, R}^{(n-1)}\right)\right)^{2} . \tag{S4}
\end{align*}
$$

As we have demonstrated in the main text, in each iteration of our algorithm, the splitting ratio $r_{m}^{(n)}$ updates according to $\left[r_{m}^{(n)}+\sum_{j} \eta\left(T_{j}-P_{j}\right) \frac{\partial P_{j}}{\partial r_{m}^{(n)}}\right] \rightarrow r_{m}^{(n)}$, where $\eta \in(0,1]$ is the learning rate and the term $\left(T_{j}-P_{j}\right)$ can be written as $e_{j}$. Since $r_{m}^{(n)}$ only connects to the two photon detector channels $P_{m-1}$ and $P_{m+1}$, the updating value of $r_{m}^{(n)}$ can be written as

$$
\begin{equation*}
\Delta r_{m}^{(n)}=\sum_{j} \eta e_{j} \frac{\partial P_{j}}{\partial r_{m}^{(n)}}=\eta\left(e_{m-1} \frac{\partial P_{m-1}}{\partial r_{m}^{(n)}}+e_{m+1} \frac{\partial P_{m+1}}{\partial r_{m}^{(n)}}\right), \tag{S5}
\end{equation*}
$$

substituting Eq. S4 into Eq. S5, we then obtain the detailed expression for the updated values of the splitting ratio $r_{m}^{(n)}$ as

$$
\begin{align*}
\Delta r_{m}^{(n)}= & \eta e_{m-1}\left[\left(\sqrt{r_{m}^{(n)}} a_{m+1, L}^{(n-1)}+\sqrt{1-r_{m}^{(n)}} a_{m-1, R}^{(n-1)}\right)\left(\frac{1}{\sqrt{r_{m}^{(n)}}} a_{m+1, L}^{(n-1)}-\frac{1}{\sqrt{1-r_{m}^{(n)}}} a_{m-1, R}^{(n-1)}\right)\right] \\
& +\eta e_{m-1}\left[( \sqrt { r _ { m } ^ { ( n ) } } b _ { m + 1 , L } ^ { ( n - 1 ) } + \sqrt { 1 - r _ { m } ^ { ( n ) } } b _ { m - 1 , R } ^ { ( n - 1 ) } ) \left(\frac{1}{\left.\left.\sqrt{r_{m}^{(n)}} b_{m+1, L}^{(n-1)}-\frac{1}{\sqrt{1-r_{m}^{(n)}}} b_{m-1, R}^{(n-1)}\right)\right]}\right.\right. \\
& +\eta e_{m+1}\left[\left(\sqrt{1-r_{m}^{(n)}} a_{m+1, L}^{(n-1)}-\sqrt{r_{m}^{(n)}} a_{m-1, R}^{(n-1)}\right)\left(-\frac{1}{\sqrt{1-r_{m}^{(n)}}} a_{m+1, L}^{(n-1)}-\frac{1}{\sqrt{r_{m}^{(n)}}} a_{m-1, R}^{(n-1)}\right)\right] \\
& +\eta e_{m+1}\left[\left(\sqrt{1-r_{m}^{(n)}} b_{m+1, L}^{(n-1)}-\sqrt{r_{m}^{(n)}} b_{m-1, R}^{(n-1)}\right)\left(-\frac{1}{\sqrt{1-r_{m}^{(n)}}} b_{m+1, L}^{(n-1)}-\frac{1}{\sqrt{r_{m}^{(n)}}} b_{m-1, R}^{(n-1)}\right)\right] . \tag{S6}
\end{align*}
$$

Therefore, during the training process of our algorithm, we iteratively update the values of $r_{m}^{(n)}$ according to Eq. 56 to minimize the loss function. For a splitting ratio in the walking step other than the last step, the derivation of its updating value in our algorithm is similar to the above process. Here we consider the splitting ratio at position $m$ in the $(n-1)$ walking step of an $n$-step quantum walk, as depicted in Fig. S1. From Fig. S1 we can see that the value of $r_{m}^{(n-1)}$ affects three photon detection probabilities: $P_{m-2}, P_{m}, P_{m+2}$. Therefore, the updating value of $r_{m}^{(n-1)}$ during the algorithm training process can be written as

$$
\begin{align*}
\Delta r_{m}^{(n-1)} & =\sum_{j} \eta e_{j} \frac{\partial P_{j}}{\partial r_{m}^{(n-1)}}=\eta\left(e_{m-2} \frac{\partial P_{m-2}}{\partial r_{m}^{(n-1)}}+e_{m} \frac{\partial P_{m}}{\partial r_{m}^{(n-1)}}+e_{m+2} \frac{\partial P_{m+2}}{\partial r_{m}^{(n-1)}}\right) . \\
& =\eta e_{m-1}\left(\frac{\partial P_{m-2}}{\partial a_{m-1, L}^{(n)}} \frac{\partial a_{m-1, L}^{(n)}}{\partial a_{m, L}^{(n-1)}} \frac{\partial a_{m, L}^{(n-1)}}{\partial r_{m}^{(n-1)}}+\frac{\partial P_{m-2}}{\partial b_{m-1, L}^{(n)}} \frac{\partial b_{m-1, L}^{(n)}}{\partial b_{m, L}^{(n-1)}} \frac{\partial b_{m, L}^{(n-1)}}{\partial r_{m}^{(n-1)}}\right) . \tag{S7}
\end{align*}
$$

The terms in brackets in Eq. S 7 are the sum of the partial derivatives of $\left\{P_{m-2}, P_{m}, P_{m+2}\right\}$ with respect to $r_{m}^{(n-1)}$, which can be split into four partial derivation paths as marked in Fig. S1(b).
(a)




Fig. S2. Numerical simulations of a Gaussian (a) and a uniform (b) probability distributions of a quantum walk system with $1 \%$ deviation in the splitting ratio. Box-plot is counted from 100 numerical simulation results. Red markers indicate the ideal probabilities of the target distributions.
distributions. The box-plots are drawn by characterizing 100 numerical simulation results. From Fig. S2 we can see that the influence caused by the splitting ratio deviation are tolerable. The fidelities of the simulated probability distributions with deviation are also above $95 \%$, which further proves the strong robustness of our quantum walk system.

