Generating pseudo-random discrete probability distributions: About the normalization and trigonometric methods

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The generation of pseudo-random discrete probability distributions is of paramount importance for a wide range of stochastic simulations spanning from Monte Carlo methods to the random sampling of quantum states for investigations in quantum information science. In spite of its significance, a thorough exposition of such a procedure is lacking in the literature. In this article we present relevant details concerning the numerical implementation of what we call the normalization and trigonometric methods for generating an unbiased probability vector $\vec{p} = (p_1, \cdots, p_d)$. An immediate application of these results regarding the generation of pseudo-random pure quantum states is also described.

I. INTRODUCTION

Roughly speaking, randomness is the fact that, even using all the information we have about a physical system, in some situations it is impossible or unfeasible for us to predict exactly the future state of the system. Randomness is a facet of nature that is ubiquitous and very influential in our and other societies [1–3]. As a consequence, it is also an essential aspect of our science and technology. The related research theme, that was motivated initially mainly by gambling and led eventually to probability theory [4, 5], is nowadays a crucial part of many different fields of study such as computational simulations, information theory, cryptography, statistical estimation, system identification, and many others [6–8].

One rapid-growing area of research for which randomness is a key concept is the maturing field of quantum information science (QIS). Our main aim in this field is understanding how quantum systems can be harnessed in order to use all Nature’s potentialities for information storage, processing, transmission, and protection [9, 10].

Quantum mechanics [11, 12] is one of the present fundamental theories of Nature. The essential mathematical object in this theory is the density operator (or density matrix) $\rho$. It embodies all our knowledge about the preparation of the system, i.e., about its state. From the mathematical point of view, a density matrix is simply a positive semi-definite matrix (notation: $\rho \geq 0$) with trace equal to one ($\text{Tr}(\rho) = 1$). Such kind of matrix can be written as $\rho = \sum_j r_j \Pi_j$, which is known as the spectral decomposition of $\rho$. In the last equation $\Pi_j$ is the projector ($\Pi_j \Pi_k = \delta_{jk} \Pi_j$ and $\sum_j \Pi_j = \mathbb{I}_d$, where $\mathbb{I}_d$ is the $d$–dimensional identity matrix) on the vector subspace corresponding to the eigenvalue $r_j$ of $\rho$. From the positivity of $\rho$ follows that, besides it being Hermitian and hence having real eigenvalues, its eigenvalues are also non-negative, $r_j \geq 0$. Once the trace function is base independent, the eigenvalues of $\rho$ must sum up to one, $\text{Tr}(\rho) = \sum_j r_j = 1$. Thus we see that the set $\{r_j\}$ possesses all the features that define a probability distribution (see e.g. Ref. [4]).

The generation of pseudo-random quantum states is an essential tool for inquires in QIS (see e.g. Refs. [13–22]) and involves two parts. The first one is the generation of pseudo-random sets of projectors $\{\Pi_j\}$, that can be cast in terms of the creation of pseudo-random unitary matrices. There are several methods for accomplishing this last task [23–26], whose details shall not be discussed here. Here we will address the second part, which is the generation of pseudo-random discrete probability distributions [27–29], dubbed here as pseudo-random probability vectors (pRPV).

In this article we go into the details of two methods for generating numerically pRPVs. In Sec. II the standard normalization method is discussed. The bias of the pRPV appearing in its naive-direct implementation is highlighted. A simple solution to this problem via random shuffling of the pRPV components is then presented. In Sec. III we consider the trigonometric method. After discussing some issues regarding its biasing and numerical implementation, we study and compare the computer time required by the two methods when the dimension of the pRPV is varied. The conclusions and prospects are presented in Sec. IV.

II. THE NORMALIZATION METHOD

By definition, a discrete probability distribution [4] is a set of non-negative real numbers,

$$p_j \geq 0,$$  \hspace{1cm} (1)

that sum up to one,

$$\sum_{j=1}^{d} p_j = 1.$$  \hspace{1cm} (2)

In this article we will utilize the numbers $p_j$ as the components of a probability vector

$$\vec{p} := (p_1, \cdots, p_d).$$  \hspace{1cm} (3)

Despite the nonexistence of consensus regarding the meaning of probabilities [4], here we can consider $p_j$ simply as the relative frequency with which a particular value

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for the cases $d=2$ (figure on the left) and $d=3$ (figure on the right). For higher dimensions the probability space is a hyperplane.

In the table below is presented the mean value of the components of $\vec{q}$ for $10^6$ pRPV generated.

$$
\begin{array}{ccccccc}
 d & \langle q_1 \rangle & \langle q_2 \rangle & \langle q_3 \rangle & \langle q_4 \rangle & \langle q_5 \rangle & \langle q_6 \rangle \\
 2 & 0.50006 & 0.49992 & 0.50001 & 0.49992 & 0.50001 & 0.49992 \\
 3 & 0.49999 & 0.25014 & 0.49999 & 0.25014 & 0.49999 & 0.25014 \\
 4 & 0.49981 & 0.12504 & 0.49981 & 0.12504 & 0.49981 & 0.12504 \\
 5 & 0.50038 & 0.06250 & 0.50038 & 0.06250 & 0.50038 & 0.06250 \\
 6 & 0.50038 & 0.03124 & 0.50038 & 0.03124 & 0.50038 & 0.03124 \\
\end{array}
$$

In the inset of Fig. 1 is shown an example with the resulting probability distributions for the four components of $\vec{q} = (q_1, q_2, q_3, q_4)$.
From the discussion above we see that in addition to the \( d - 1 \) pRN needed for the biased pRPV, we have to generate more \( d - 1 \) pRN for the shuffling used in order to obtain an unbiased pRPV (because \( \sum_{j=1}^{d} j = d(d+1)/2 \)), resulting in a total of \( 2(d - 1) \) pRN per pRPV.

III. THE TRIGONOMETRIC METHOD

As the name indicates, this method uses a trigonometric parametrization \([27, 29]\) for the components of the probability vector \( p = (p_1, \ldots, p_d) \):

\[
p_j := \sin^2 \theta - 1 \prod_{k=j}^{d-1} \cos^2 \theta_k,
\]

with \( \theta_0 = \pi/2 \) (so the name trigonometric method). More explicitly,

\[
p_1 = \sin^2 \theta_0 \cos^2 \theta_1 \cos^2 \theta_2 \cos^2 \theta_3 \cdots \cos^2 \theta_{d-1}
p_2 = \sin^2 \theta_1 \cos^2 \theta_2 \cos^2 \theta_3 \cdots \cos^2 \theta_{d-1}
p_3 = \sin^2 \theta_2 \cos^2 \theta_3 \cos^2 \theta_4 \cdots \cos^2 \theta_{d-1}
\]

\[
\vdots
\]

\[
p_{d-1} = \sin^2 \theta_{d-2} \cos^2 \theta_{d-1}
p_d = \sin^2 \theta_{d-1}.
\]

A simple application of the trigonometric equality \( \cos^2 \theta_j + \sin^2 \theta_j = 1 \) to this last equation shows that \( p_j \geq 0 \) and \( \sum_{j=1}^{d} p_j = 1 \). Therefore this parametrization, which utilizes \( d - 1 \) angles \( \theta_j \), leads to a well defined probability distribution \( \{p_j\}_{j=1}^{d} \).

Let us regard the numerical generation of a unbiased pseudo-random probability vector by starting with the parametrization in Eq. (5). For generating an uniform pRPV we can proceed as follows. We begin with \( p_d \) and go all the way to \( p_1 \) imposing that each \( p_j \) must be uniformly distributed in \([0, 1]\). Thus we must have

\[
\theta_{d-1} = \arcsin \sqrt{t_{d-1}}
\]

and the other angles \( \theta_j \), with \( j = 1, \ldots, d - 2 \), should be generated as shown in the next equation:

\[
\theta_j = \arcsin \sqrt{\frac{t_j}{\prod_{k=j+1}^{d-1} \cos^2 \theta_k}}.
\]

where \( t_j \), with \( j = 1, \ldots, d - 1 \), are pseudo-random numbers with uniform distribution in the interval \([0, 1]\). For obvious reasons, this manner of generating a pRPV is very unstable, and therefore inappropriate, for numerical implementations.

A possible way out of this nuisance is simply to ignore the squared cosines in the denominator of Eq. (9). That is to say, we may generate the angles using

\[
\theta_j = \arccos \sqrt{t_j}
\]

for all \( j = 1, \ldots, d - 1 \). This procedure will give us an uniform distribution for \( \cos^2 \theta_j \) and \( \sin^2 \theta_j \), but will also increase the chance for the components \( p_j \) with more terms to have values closer to zero. Thus, there is the issue of a biased pRPV again. A possible solution for this problem is, once more, shuffling. In the next two tables are shown the average value of the components of \( 10^6 \) pRPV generated via the trigonometric method before, \( \langle p_j \rangle \),

\[
\begin{array}{cccccccc}
\text{d} & \langle p_1 \rangle & \langle p_2 \rangle & \langle p_3 \rangle & \langle p_4 \rangle & \langle p_5 \rangle & \langle p_6 \rangle \\
2 & 0.49987 & 0.50013 & & & & \\
3 & 0.25023 & 0.24973 & 0.49994 & & & \\
4 & 0.12497 & 0.12507 & 0.24967 & 0.50029 & & \\
5 & 0.06249 & 0.06235 & 0.12502 & 0.24955 & 0.50058 & \\
6 & 0.03128 & 0.03134 & 0.06265 & 0.12483 & 0.24987 & 0.50002 \\
\end{array}
\]

and after, \( \langle q_j \rangle \), shuffling.

\[
\begin{array}{cccccccc}
\text{d} & \langle q_1 \rangle & \langle q_2 \rangle & \langle q_3 \rangle & \langle q_4 \rangle & \langle q_5 \rangle & \langle q_6 \rangle \\
2 & 0.50063 & 0.49937 & & & & \\
3 & 0.33299 & 0.33336 & 0.33365 & & & \\
4 & 0.29011 & 0.24972 & 0.25011 & 0.24999 & & \\
5 & 0.20049 & 0.19978 & 0.19991 & 0.20008 & 0.19974 & \\
6 & 0.16664 & 0.16649 & 0.16669 & 0.16682 & 0.16704 & 0.16632 \\
\end{array}
\]

As was the case with the normalization method, for the trigonometric method we need to generate \( 2(d - 1) \) pRN per pRPV, \( d - 1 \) for the angles and \( d - 1 \) for the random permutation. Nevertheless, because of the additional multiplications in Eq. (5), the computation time for the last method is in general a little greater than that for the former, as is shown in Fig. 3.

IV. CONCLUDING REMARKS

In this article we discussed thoroughly two methods for generating pseudo-random discrete probability distributions. We identified some difficulties for the numerical
implementation of the trigonometric method. The fact that in a direct application of both the normalization and trigonometric methods one shall generate biased probability vectors was emphasized. Then the shuffling of the pseudo-random probability vector components was shown to solve this problem at the cost of the generation of additional \( d - 1 \) pseudo-random numbers for each pRPV.

It is worthwhile recalling that pure quantum states in \( \mathbb{C}^d \) can be written in terms of the computational basis \( \{|c_j\rangle\}_{j=1}^d \) as follows:

\[
|\psi\rangle = \sum_j c_j |c_j\rangle = \sum_j |c_j| e^{i\phi_j} |c_j\rangle = \sum_j \sqrt{p_j} e^{i\phi_j} |c_j\rangle, \tag{11}
\]

where \( c_j \in \mathbb{C} \) and \( \phi_j \in \mathbb{R} \). The normalization of \( |\psi\rangle \) implies that the set \( \{p_j\} \) is a probability distribution. Thus the results reported in this article are seem to have a rather direct application for the generation of unbiased pseudo-random state vectors.

We observe however that the content presented in this article can be useful not only for the generation of pseudo-random quantum states in quantum information science, but also for stochastic numerical simulations in other areas of science. An interesting problem for future investigations is with regard to the possibility of decreasing the number of pRN, and thus the computer time, required for generating an unbiased pRPV. In the Appendix A we discuss a method that uses only \( d \) pRN per pRPV and show that it presents a crucial problem which prevents its use.

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Appendix A: The iid method

A simple way to generate an unbiased pseudo-random probability vector \( \vec{p} = (p_1, \cdots, p_d) \) is as follows. If we create \( d \) independent pseudo-random numbers \( x_j \) with identical probability distributions in the interval \([0, 1]\) (so the name of the method) and set \( p_j := x_j / \sum_{k=1}^d x_k \), we will obtain a well defined discrete probability distribution, i.e., \( p_j \geq 0 \) and \( \sum_{j=1}^d p_j = 1 \). Besides, one can verify that the mean value of \( p_j \) approaches \( 1/d \) as the number of samples grows.

Nevertheless, the sum \( \sum_{k=1}^d x_k \) shall be typically greater than one. This in turn will lead to the impossibility for the occurrence of pRPVs with one of its components equal (or even close) to one. As can be seen in Fig. 4, this problem becomes more and more important as \( d \) increases. Therefore, this kind of drawback makes impossible the application of the iid method for the task regarded in article.

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