Simulating sparse and shallow Gaussian Boson Sampling

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Abstract. Gaussian Boson Sampling (GBS) is one of the most popular quantum supremacy protocols as it does not require universal control over the quantum system, which favors current photonic experimental platforms and there is strong theoretical evidence for its computational hardness. However, over the years, several algorithms have been proposed trying to increase the performance of classically simulating GBS assuming certain constraints, e.g., a low number of photons or shallow interferometers. Most existing improvements of the classical simulation of GBS provide a performance increase regarding the probability calculation, leaving the sampling algorithm itself untouched. This paper provides an asymptotically better sampling algorithm in the case of low squeezing and shallow circuits.

Keywords: Quantum Computing · Quantum Computer Simulation · Quantum Advantage

1 Introduction

In the last decade, photonic quantum computing has gained more relevance in the quantum computing world due to its apparent scalability and the recent demonstration of photonic quantum advantage [17]. In particular, in recent experiments, the so-called Gaussian Boson Sampling (GBS) scheme was used in recent experiments to demonstrate that photonic quantum devices are capable of solving a classically hard task [16]. This sampling schemes has also been demonstrated to have several special applications, e.g., in graph problems [2] and quantum chemistry [3]. Therefore, trying to improve algorithms for simulating GBS has gained attraction.

Simulation of GBS is also a necessary step in creating a photonic quantum computer, since quantum computer manufacturers need to compare experimen-

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tal data with a simulation for assessing inaccuracies. Moreover, an efficient simulation algorithm enables researchers to be able to perform various numerical experiments on a classical computer testing new quantum protocols.

In its essence, GBS means the mode-wise photon detection of a multimode Gaussian state [9,10]. The scheme can be simulated by calculating the probabilities of the photon detection events using the displacement vector and covariance matrix of the Gaussian state. However, the probabilities turn out to be classically hard (#P-hard) to compute in general and there is also theoretical evidence that sampling from this distribution is hard [8], hence an existing photonic quantum computer has an advantage over classical computers.

One feature that makes the direct simulation of GBS hard is the size of the event space. The number of photon detection events exponentially increases in the number of modes, repeating the calculation of the probabilities many times. To counter this problem, one can introduce a mode-by-mode sampling algorithm which does not calculate the probabilities for all the possible events, but only for a certain subset of the sample space, hence reducing the complexity of the calculation [12].

The complexity of the (loop) hafnian is at the heart of the classical simulation of GBS. The state-of-the-art algorithm for calculating this quantity is the power trace method introduced by Björklund et al. [5]. Additionally, one could achieve a considerable speedup by modifying the original mode-by-mode sampling algorithm, described by Quesada et al. [12]. In their paper, they achieved a quadratic speedup over the original particle-resolved GBS algorithm, using the fact that the formula of (loop) hafnian for Gaussian pure states simplifies [14].

Since the inception of GBS, several algorithms have been proposed to simulate certain edge cases more efficiently [11,4]. Important edge cases are, e.g., when the Gaussian states have relatively low average particle numbers (sparse circuit) or when the interferometer used in the production of the Gaussian state is shallow. In the sparse and shallow case, a faster algorithm for calculating the (loop) hafnian has been already proposed [11], but a modification of the sampling algorithm in this scenario has not been considered before. Therefore, we propose an algorithm for simulating GBS for sparse and shallow photonic Gaussian circuits.

The structure of the paper is as follows: in Section 2 the basics of the GBS scheme are introduced. In Section 3 the proposed sampling algorithm is derived and introduced. Lastly, in Section 4, the complexity of the algorithm is calculated in the case of non-displaced threshold GBS.

2 Setup

In this section, basic familiarity with quantum optics and photonic Gaussian states is assumed. For reference, the reader may visit Refs. [1,15].

A d-mode Gaussian state ρ can be completely characterized by its displacement vector $\bar{r} = \operatorname{tr}[\hat{r}\rho]$ and covariance matrix $\sigma = \frac{1}{2}\operatorname{tr}[\{\hat{r} - \bar{r}, \hat{r} - \bar{r}\}\rho]$, where

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$\hat{r} = (x_1, \ldots, x_d, p_1, \ldots, p_d)$ is the vector containing the x_i, p_i quadrature operators, and $\{A, B\}$ denotes the anticommutator of the operators A and B .

Gaussian states can be similarly characterized by their complex displacement vector and their Q-function covariance matrix

$$\gamma = \mathrm{tr}\left[\xi\rho\right], \tag{1}$$

$$\Sigma = \frac{1}{2}\left(\mathrm{tr}\left[\{(\xi-\gamma),(\xi-\gamma)^\dagger\}\rho\right] + \mathbb{1}\right), \tag{2}$$

where $\xi = (a_1, \ldots, a_d, a_1^\dagger, \ldots, a_d^\dagger)$ is the vector containing the creation and annihilation operators.

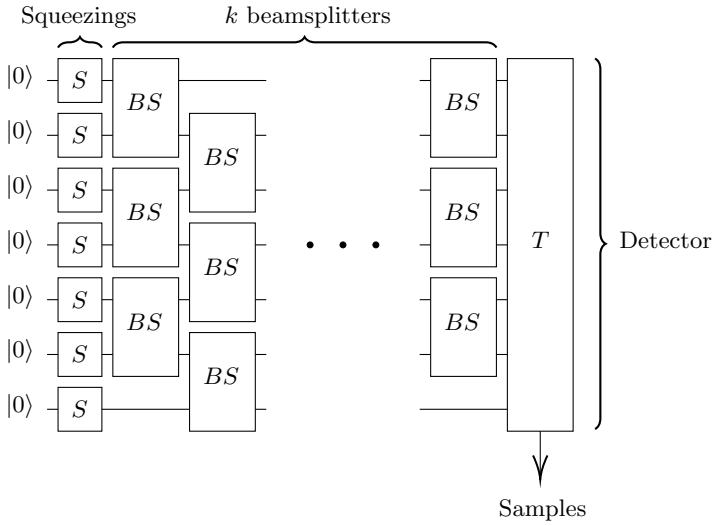

Fig. 1. The basic setup of GBS without displacement. On the vacuum state, a column of squeezings is applied with different squeezing parameters, and then k column of beamsplitters with alternating starting positions depending on the parity of the column, as demonstrated by the diagram.

In the most usual variant of the GBS scheme one performs a mode-wise photon number detection measurement, which is a projective measurement described by the projections

$$P_n = |n\rangle\langle n| \qquad (n \text{ photon}, n \in \mathbb{N}_0). \tag{3}$$

One can easily specialize towards a coarser detection scheme, the so called *threshold detection*. The threshold detection measurement for one mode is defined by

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projections

$$Q_0 = P_0 = |0\rangle\langle 0| \qquad \text{(0 photon)},$$
$$Q_1 = \sum_{n=1}^{\infty} P_n = \mathbb{1} - Q_0 \qquad (\geq 1 \text{ photons, click}). \tag{4}$$

On multiple modes, the tensor product of the one-mode projection elements define measurement projections

$$\{R_{s_1} \otimes \cdots \otimes R_{s_d}\}_{(s_1,\ldots,s_d)\in I^d} =: \{R_S\}_{S\in I^d}\,, \tag{5}$$

where I could either denote $\{0,1\}$ or $\mathbb{N}_0 = \{0,1,2,\dots\}$ and R_S could denote either P_S or Q_S, and d is the number of modes. Given a quantum state ρ, the probability of detecting the sample $S \in I^d$ is

$$p(S) = \operatorname{tr}\left[\rho R_S\right]. \tag{6}$$

Consider a d-mode Gaussian state with complex displacement vector γ and Q-function covariance matrix Σ. An important observation is that in GBS the probability of detecting a sample $S \in I^d$ can be multiplicatively factorized to a function which depends on $S, \operatorname{br}_S \gamma, \operatorname{br}_S \Sigma^{-1}$ only, and a second function which depends purely on Σ, γ. More concretely, one can write

$$p(S) = N(\gamma,\Sigma) f\left(S, \operatorname{br}_S \gamma, \operatorname{br}_S \Sigma^{-1}\right), \tag{7}$$

where br_S denotes the block-wise repetition of rows and columns by S (0 entry means elimination of the row or column); for the formal definition see Appendix A. The calculation of f is usually a classically hard task, and N is just a normalization factor, independent of the sample S, fulfilling the following block matrix factorization property:

$$N(\gamma_1 \oplus_b \gamma_2, \Sigma_1 \oplus_b \Sigma_2) = N(\gamma_1,\Sigma_1) N(\gamma_2,\Sigma_2). \tag{8}$$

Probability expressions of the form of Eq. (7) are motivated by several GBS-related sampling schemes, where the function f contains the (loop) torontonian [6] or (loop) hafnian [5]. As a simple example, for a Gaussian state 0 complex displacement vector and Q-function covariance matrix Σ, the threshold detection probability can be calculated by the formula

$$p(S) = \frac{\operatorname{tor}\left(\operatorname{br}_S O\right)}{\sqrt{\det\left(\Sigma\right)}}, \tag{9}$$

where $O = \mathbb{1} - \Sigma^{-1}$ and tor denotes the torontonian [13]. Naively, to sample from the probability distribution one would need to calculate the probability for all elements in the sample space $\Omega = \{S \in I^d\}$. Since $|\Omega| = |I|^d$ scales exponentially in the number of modes d, the sampling algorithm constructed in this fashion may be computationally demanding in general. Instead, one can opt for a sampling method where knowledge of all the probabilities is not necessary. For the simulation of photonic quantum computing, the mode-by-mode sampling method is used extensively, which is introduced by Quesada et al. [13] for the case of non-displaced threshold GBS.

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3 Classical simulation of sparse and shallow GBS

In this section, we would like to introduce a classical algorithm which may have better performance than previous algorithms in the case of low particle numbers (sparse) and shallow interferometers. A key observation is that the (loop) torontonian and (loop) hafnian functions factorize over block direct sum due to Theorem 3 in Appendix B. The following question arises: can the mode-by-mode algorithm be improved using Theorem 3? The answer turns out to be positive, as demonstrated in this section.

Consider a d-mode photonic quantum system according to Figure 1 with k beamsplitter columns. Let $r = (r_1, \ldots, r_d) \in \mathbb{R}_+^d$ squeezing parameters corresponding to the squeezing gates and $U \in U(d)$ unitary matrix corresponding to the interferometer consisting of the beamsplitters. Then the Q-function covariance matrix of the state before threshold detection is

$$\Sigma = \begin{bmatrix} U & \\ & U^* \end{bmatrix} \begin{bmatrix} \cosh^2 r & \cosh r \sinh r \\ \cosh r \sinh r & \cosh^2 r \end{bmatrix} \begin{bmatrix} U^\dagger & \\ & U^T \end{bmatrix}. \tag{10}$$

The unitary $U \in U(d)$ corresponding to the columns of beamsplitters can get "banded" if the number of beamsplitter columns k is smaller than d. To properly formulate this, we need the definition of bandwidth:

Definition 1 (Set of k-bandwidth matrices). *The set of k-bandwidth matrices is*

$$\mathrm{Band}_k(\mathbb{C}^{n\times n}) := \left\{ A \in \mathbb{C}^{n\times n} \mid \forall i \in [n] : \begin{cases} \text{if } i < n-k : \forall a \in [n-i-k] : A_{i,i+k+a} = 0 \\ \text{if } i > k : \forall a \in [i-k] : A_{i,i-k-a} = 0 \end{cases} \right\}. \tag{11}$$

For convenience, let us define a function which assigns the minimal number of matching row and column eliminations to decompose the "overestimated" matrix to direct sums of smaller matrices.

Definition 2. *Let $n \in \mathbb{N}_+$ and let $A \in \mathbb{C}^{n\times n}$. The function* band : $\mathbb{C}^{n\times n} \to \mathbb{N}$ *is defined as*

$$A \mapsto \min_{k\in[n]} \left\{ k : A \in \mathrm{Band}_k(\mathbb{C}^{n\times n}) \right\} \tag{12}$$

Consider a d-mode circuit of $m \leq d/2$ columns of beamsplitters, and denote the interferometer of each column by $U_i \in U(d), 1 \leq i \leq m$. One can easily show that the bandwidth of $U := U_1 \ldots U_m$ is just m, i.e. $\mathrm{band}(U_1 \ldots U_m) = m$, and hence $\mathrm{band}(\Sigma) = 2m =: k$. Therefore, for circuits where $\mathrm{band}(\Sigma) < d$, one can have occurrences during the sampling procedure when the reduction bitstring S has 0-substrings of length k and using Theorem 3, the probabilities would factorize. More concretely, define a bitstring S by concatenating two arbitrary bitstring S_1, S_2 by k 0s, i.e. let $S = S_1 0^k S_2$. Moreover, let $n = |S|$ and consider

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a matrix $M \in \mathbb{C}^{2n\times 2n}$ which can be decomposed into $A, B, C, D \in \mathbb{C}^{n\times n}$ blocks, i.e.

$$M = \begin{bmatrix} A & B \\ C & D \end{bmatrix} \tag{13}$$

such that $\mathrm{band}(A) = \mathrm{band}(B) = \mathrm{band}(C) = \mathrm{band}(D) = k$. Then we can write

$$\mathrm{br}_S\, M = \begin{bmatrix} A_1 \oplus A_2 & B_1 \oplus B_2 \\ C_1 \oplus C_2 & D_1 \oplus D_2 \end{bmatrix} =: M_1 \oplus_b M_2, \tag{14}$$

where - again - the bandwidth of every submatrix is k. In Theorem 3 it has already been shown, that the part of the probability which depends on the sample S factorizes over block direct sums. A natural question would be whether one could use this formula in the mode-by-mode sampling algorithm. One could immediately note that factorizing is not a trivial matter, since in the algorithm, the Q-function covariance matrix is block reduced for each iteration by the first n modes. In each iteration indexed by n, the $(\mathrm{r}_{1^n0^{d-n}}\, \Sigma)^{-1}$ matrix is calculated, which is different for each iteration. This matrix then needs to be reduced again by the previous samples to calculate probability, according to Eq (7). If one could interchange the inversion on Σ and the first reduction by 1^n0^{d-n}, Theorem 3 could be trivially used to factorize in the algorithm whenever a 0^k substring appears in the sample, but it is not entirely obvious if such interchange of operations is permitted. Luckily, the following theorem asserts that this is indeed the case:

Theorem 1. *Let $\Sigma \in \mathbb{C}^{2d\times 2d}$ be the Q-function covariance matrix for a pure Gaussian state in which the interferometer matrix $U \in U(d)$ is m-bandwidth and $r = (r_1, \ldots, r_d) \in \mathbb{R}^d_{\geq 0}$. Let $k = 2m$, $k \leq n \leq d$, $S = 1^{(n-k)}0^k$ and $F = 1^n0^{(d-n)}$. Then*

$$(\mathrm{br}_S \circ \mathrm{inv} \circ \mathrm{br}_F)\, \Sigma = (\mathrm{br}_S \circ \mathrm{br}_F \circ \mathrm{inv})\, \Sigma = \mathrm{br}_S\, \mathrm{br}_F \left(\Sigma^{-1}\right). \tag{15}$$

Proof. By direct computation one gets

$$\mathrm{br}_S\, \mathrm{br}_F \left(\Sigma^{-1}\right) = \begin{bmatrix} \mathbb{1} & -\mathrm{r}_S\, \mathrm{r}_F\, B \\ -\mathrm{r}_S\, \mathrm{r}_F\, B^* & \mathbb{1} \end{bmatrix}, \qquad \Sigma^{-1} = \begin{bmatrix} \mathbb{1} & -B \\ -B^* & \mathbb{1} \end{bmatrix}, \tag{16}$$

where $B := U \tanh(r) U^T \in \mathbb{C}^{d\times d}$, which is equivalent to the result of Proposition 4 from Appendix C. □

Let $\Sigma \in \mathbb{C}^{2d\times 2d}$ have k-bandwidth submatrices as before. Let S_1 and S_2 be arbitrary bitstrings, and let $n := |S_1| + |S_2| + k \leq d$. Then

$$\mathrm{br}_{S_1 0^k S_2}\, \Sigma^{-1} = \mathrm{br}_{S_1 0^k S_2}\, \Sigma^{-1} = \mathrm{br}_{S_1 0^k 0^{|S_2|}}\, \Sigma^{-1} \oplus_b \mathrm{br}_{0^{|S_1|} 0^k S_2}\, \Sigma^{-1}, \tag{17}$$

where using Theorem 1 we can write

$$\mathrm{br}_{S_1 0^k 0^{|S_2|}}\, \Sigma^{-1} = (\mathrm{br}_{S_1 0^k} \circ \mathrm{inv} \circ \mathrm{br}_{1^{|S_1|} 1^k 0^{|S_2|}})\Sigma, \tag{18}$$

$$\mathrm{br}_{0^{|S_1|} 0^k S_2}\, \Sigma^{-1} = (\mathrm{br}_{0^k S_2} \circ \mathrm{inv} \circ \mathrm{br}_{0^{|S_1|} 1^k 1^{|S_2|}})\, \Sigma, \tag{19}$$

$$\begin{aligned} \mathrm{br}_{S_1 0^k S_2}\, \Sigma^{-1} = {} & (\mathrm{br}_{S_1 0^k} \circ \mathrm{inv} \circ \mathrm{br}_{1^{|S_1|} 1^k 0^{|S_2|}})\, \Sigma \\ & \oplus_b (\mathrm{br}_{0^k S_2} \circ \mathrm{inv} \circ \mathrm{br}_{0^{|S_1|} 1^k 1^{|S_2|}})\, \Sigma. \end{aligned} \tag{20}$$

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Putting it all together, it is apparent that we can cut the mode-by-mode sampling at a 0^k pattern. Finally, using Theorem 3 we conclude that

$$\begin{aligned} & f(S_1 0^k S_2, \mathrm{br}_{S_1 0^k S_2}\, \gamma, \mathrm{br}_{S_1 0^k S_2}\, \Sigma^{-1}) \\ & \quad = f(S_1 0^k, \mathrm{br}_{S_1 0^k}\, \mathrm{br}_{1^{|S_1|} 1^k 0^{|S_2|}}\, \gamma, \mathrm{br}_{S_1 0^k}(\mathrm{br}_{1^{|S_1|} 1^k 0^{|S_2|}}\, \Sigma^{-1})) \\ & \quad \times f(0^k S_2, \mathrm{br}_{0^k S_2}\, \mathrm{br}_{0^{|S_1|} 1^k 1^{|S_2|}}\, \gamma, \mathrm{br}_{0^k S_2}(\mathrm{br}_{0^{|S_1|} 1^k 1^{|S_2|}}\, \Sigma^{-1})), \end{aligned} \tag{21}$$

which means that when at least k zeroes are encountered, the Q-function covariance matrix Σ will be factorized during the sampling algorithm. More concretely, the terms in the product are independent of S_1 and S_2 respectively, so during the sampling algorithm where the S_2 sample is varied for calculating the probability distribution, the first term dependent on S_1 will not change. Furthermore, one can also omit to calculate the normalization factor N and keep track of the probability from the previous sampling for calculating conditional probability.

In particular, for the case of non-displaced Gaussian Threshold Boson Sampling, one can write

$$\begin{aligned} (\mathrm{tor} \circ \mathrm{br}_{S_1 0^k S_2})\,(\mathbb{1} - \Sigma^{-1}) = \mathrm{tor}\, \mathrm{br}_{S_1 0^k} \left(\mathbb{1} - (\mathrm{br}_{1^{|S_1|} 1^k 0^{|S_2|}}\, \Sigma)^{-1}\right) \\ \times \mathrm{tor}\, \mathrm{br}_{0^k S_2} \left(\mathbb{1} - (\mathrm{br}_{0^{|S_1|} 1^k 1^{|S_2|}}\, \Sigma)^{-1}\right), \end{aligned} \tag{22}$$

and using all these insights, one can build an algorithm which could be seen in Algorithm 1. In this algorithm, when a 0^k substring appears in the samples, the input of the torontonian function can be factorized, and it is sufficient to consider only a subsystem which starts from the beginning of the 0^k substring in the sample. The non-displaced threshold GBS is emphasized because one could give an upper bound for its average complexity, discussed in the following section.

Algorithm 1 Proposed non-displaced threshold GBS algorithm for small-depth interferometer

Require: Q-function covariance matrix Σ, bandwidth k
  $d \leftarrow \dim \Sigma/2$
  $S, A \leftarrow []$ ▷ Empty list for samples and accumulator
  while $|S| + |A| < d$ **do**
    $n \leftarrow |A| + 1$
    if $|S| = 0$ **then**
      $F \leftarrow 1^n 0^{d-n}$
      $S_0 \leftarrow S + [0]$
      $S_1 \leftarrow S + [1]$
    else
      $F \leftarrow 0^{|S|-k} 1^{k+n} 0^{d-n-|S|}$
      $S_0 \leftarrow 0^k + S + [0]$
      $S_1 \leftarrow 0^k + S + [1]$
    end if
    $w_0 \leftarrow N\ \mathrm{tor}(\mathrm{br}_{S_0}(\mathbb{1} - \mathrm{br}_F(\Sigma)^{-1}))$ ▷ 0-detection weight
    $w_1 \leftarrow N\ \mathrm{tor}(\mathrm{br}_{S_1}(\mathbb{1} - \mathrm{br}_F(\Sigma)^{-1}))$ ▷ 1-detection weight
    $c \leftarrow$ choose from $(0, 1)$ with weights (w_0, w_1)
    $S \leftarrow S + [c]$
    if last k elements in S are all 0s **then**
      $A \leftarrow A + S$
      $S \leftarrow []$ ▷ Sample is emptied
    end if
  end while

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4 Complexity of the classical algorithm for non-displaced Gaussian Threshold Boson Sampling

According to the proposed Algorithm 1, the size of the matrices serving as inputs of the torontonian can be reduced, since the sample S is emptied when a 0^k bitstring is encountered in the sample. To give an upper bound for the complexity of the algorithm, one is required to find a lower bound for the vacuum detection probability, given a set of squeezing parameters.

Theorem 2 (Lower bound for vacuum probability). *Let G_r^d be the set of d-mode pure non-displaced Gaussian states with squeezing parameters $r = (r_1, \ldots, r_d)$, and $S \in P([d])$ a set containing mode numbers. Then*

$$\inf_{\rho \in G_r^d} p_\rho^S(0) \geq \cosh^{-2|S|} \max_{i \in [d]} r_i, \tag{23}$$

where $p_\rho(S = 0)$ is the probability of detecting vacuum on modes defined by S.

Proof. For a non-displaced Gaussian state, the vacuum probability can be calculated by $p_\rho^S(0) = \det\left[\mathrm{br}_S\, \Sigma_\rho\right]^{-\frac{1}{2}}$, where Σ_ρ is the Q-function covariance matrix corresponding to ρ. Hence, one needs to calculate

$$\inf_{\rho \in G_r^d} p_\rho^S(0) = \sup_{U \in U(d)} \det\left[\mathrm{br}_S\, \Sigma\right]^{-\frac{1}{2}}.$$

According to Eq. (10), for pure Gaussian states the Q-function covariance matrices only depend on the squeezing parameters r and the interferometer U, i.e., $\Sigma = \Sigma(r, U)$. Since the squeezing parameters r are fixed, one can restate the previous optimization over states as an optimization over unitary matrices as

$$\sup_{\rho \in G_r^d} \det\left[\mathrm{br}_S\, \Sigma_\rho\right] = \sup_{U \in U(d)} \det\left[\mathrm{br}_S\, \Sigma(r, U)\right]. \tag{24}$$

If A is a positive semi-definite matrix, then $\det A \leq \left(\frac{\mathrm{Tr}\, A}{\dim A}\right)^{\dim A}$, from the arithmetic mean-geometric mean inequality. Using this relation, one can provide an upper bound for $\det\left[\mathrm{br}_S\, \Sigma\right]$. Let $r_{\max} = \max_{i \in [d]} r_i$ and write

$$\begin{aligned} \sup_{U \in U(d)} \det\left[\mathrm{br}_S\, \Sigma\right] &\leq \sup_{U \in U(d)} \left[\frac{1}{|S|} \sum_{s \in S} \left(\sum_{j=1}^{d} u_{sj} u_{sj}^* \cosh^2 r_j\right)\right]^{2|S|} \\ &= \cosh^{4|S|} r_{\max}. \end{aligned} \tag{25}$$

□

Using Theorem 2, one can bound the probability distribution p_ρ^S from below by an i.i.d. probability distribution p as

$$p_\rho^S(0) \geq p(0)^{|S|} = \cosh^{-2|S|} r_{\max}, \tag{26}$$

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where $p(0)$ is the lower bound for the probability of detecting vacuum on the single mode S_i, and the corresponding probability distribution is

$$p(0) = \cosh^{-2} r_{\max}, \qquad p(1) = 1 - p(0), \tag{27}$$

which yields an i.i.d. probability distribution over all modes in S.

To give an estimate of the average complexity of Algorithm 1, we need a probability distribution which gives the probability of detecting n many 1s between 2 bitstrings of the form 0^k. For example, one could consider the bitstring

$$\underbrace{0000}_{k\ 0\text{s}}\underbrace{1011000010011}_{n=6\ 1\text{s}}\underbrace{0000}_{k\ 0\text{s}}, \tag{28}$$

where 6 1s are found between two 0^k substrings, and in this section, we will refer to these as *clusters*. Suppose that the probability of detecting 0 is uniform and independent for all modes, and denote this probability p. To generate bitstring beginning and ending with a 1, we can write

$$G = 1T + 1\left(\sum_{i=0}^{k-1} 0^i\right) G. \tag{29}$$

This recursion could be used to generate many other quantities, e.g., probabilities, by formally replacing 1 and 0 in the formula. For this reason, we replace $1 \mapsto z(1-p)$ and $0 \mapsto p$, where we included a parameter z in 1 since we only want to count the 1s in the bitstring (the 0s do not increase the complexity). The resulting equation can be solved for $G := G(z)$ as

$$G(z) = \frac{1-p}{z^{-1} - 1 + p^k}, \tag{30}$$

which is to be interpreted as the generator for the probability distribution for detecting 1s. However, $G(z)$ is not normalized in the sense that the coefficients of $G(z)$ would not sum up to 1, therefore one has to normalize it to yield a proper probability distribution. After normalization and expansion, we acquire

$$\hat{G}(z) := \frac{G(z)}{G(1)} = \frac{p^k}{z^{-1} - 1 + p^k} = \sum_{n=1}^{\infty} z^n p_c(n), \tag{31}$$

where $p_c(n) = p^k(1-p^k)^{n-1}$ represents the probability of encountering n 1s between two 0^k substrings. With the knowledge of this probability distribution, it is a trivial matter to calculate the average number of 1s between two 2 0^k substrings and is given by $\mathbb{E}[n] = p^{-k}$. The lower bound given by Eq. (27) is a probability distribution which is uniform and independent over all modes and using $p(0) = p$ one can write

$$\mathbb{E}[n] = (\cosh \max_i r_i)^{2k}, \tag{32}$$

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which gives an upper bound for the number of 1s in terms of the maximal squeezing parameter.

To calculate the complexity of Algorithm 1, one needs to use the complexity for the torontonian itself. It should be emphasized, that the underlying method of calculating the torontonian can be chosen freely. Suppose that the calculation of the torontonian has exponential complexity and write $\mathcal{C}_{\text{tor}} = N^{\alpha}\beta^{N}$, where $\alpha, \beta > 1$. One can give an upper bound to the complexity of a cluster of n 1s as

$$\mathcal{C}_{\text{cluster}}(n) = \sum_{N=1}^{n} N^{\alpha}\beta^{N} \leq n^{\alpha+1}\beta^{n}, \tag{33}$$

which can be used to give an upper bound for the average complexity of the cluster

$$\mathbb{E}[\mathcal{C}_{\text{cluster}}] \leq \sum_{n=1}^{\infty} p_c(n) n^{\alpha+1}\beta^{n} = \frac{p^k}{1-p^k} \sum_{n=1}^{\infty} n^{\alpha+1}[\beta(1-p^k)]^{n}, \tag{34}$$

and this expression is convergent when $p^k > 1 - \beta^{-1}$.

In summary, the complexity of the problem reduces in the proposed algorithm when a 0-substring is encountered with a certain length, which is not considered in the original threshold GBS algorithm presented in [13]. Hence, the presented sampling algorithm is faster in general for sparse and shallow circuits. It should also be noted, that the speedup presented in this section is just an illustration of the main principle of the proposed algorithm. One could simulate threshold GBS using (loop) hafnians which have lower complexity than the original algorithm [14,7], but the main principle of the proposed algorithm is applicable in these algorithms as well.

5 Conclusion and Outlook

A modified classical algorithm has been given for simulating Gaussian Boson Sampling, which takes into account the shallowness of the circuit and the low number of particles in the system. The algorithm can be applied for the threshold and the particle-resolved GBS as well, and the average complexity of the proposed algorithm has been calculated in the case of non-displaced threshold GBS.

The proposed sampling algorithm can also be employed in Gaussian Boson Sampling with photon number resolving measurements and even using displaced states. However, calculating the average complexity needs further investigation in these cases, since the calculation is not feasible by using similar assumptions as for the Threshold Gaussian Boson Sampling using torontonian. Moreover, the case of mixed Gaussian states has not been considered during this work, and it is still an open question whether the proposed algorithm is still valid in this case. This problem has been set aside for a future project.

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A Matrix operations

There are several notations regarding matrix operations throughout the article, and this section aims to collect all of them to avoid confusion.

Definition 3 (Row reduction). *Let $A \in \mathbb{C}^{n\times m}$ and let $S \in \mathbb{N}_0^n$ be a bitstring with $k := \sum_{i=0}^{|S|} S_i$. Then the row reduction $\mathrm{rr}_S : \mathbb{C}^{n\times m} \to \mathbb{C}^{k\times m}$ is the function mapping A to a matrix formed by repeating the i-th row of A S_i many times.*

Definition 4 (Column reduction). *Let $A \in \mathbb{C}^{n\times m}$ and let $S \in \mathbb{N}_0^n$ be a bitstring with $k := \sum_{i=0}^{|S|} S_i$. Then the column reduction $\mathrm{cr}_S : \mathbb{C}^{n\times m} \to \mathbb{C}^{n\times k}$ is defined by $\mathrm{cr}_S(A) := \mathrm{rr}_S(A^T)^T$.*

Definition 5 (Reduction). *Let $A \in \mathbb{C}^{n\times n}$ and let $S \in \mathbb{N}_0^n$ be a bitstring with k 1s. Then the reduction $\mathrm{r}_S : \mathbb{C}^{n\times n} \to \mathbb{C}^{k\times k}$ is defined by $\mathrm{r}_S := \mathrm{rr}_S \circ \mathrm{cr}_S$.*

Definition 6 (Block reduction). *Block reduction can only be defined on an even-dimensional matrix $M \in \mathbb{C}^{2n\times 2n}$. Let $A, B, C, D \in \mathbb{C}^{n\times n}$ and $S \in \mathbb{N}_0^n$. Then*

$$\mathrm{br}_S \begin{bmatrix} A & B \\ C & D \end{bmatrix} = \begin{bmatrix} \mathrm{r}_S A & \mathrm{r}_S B \\ \mathrm{r}_S C & \mathrm{r}_S D \end{bmatrix}. \tag{35}$$

Definition 7 (Block direct sum). *Let $n, m \in \mathbb{N}^+$, $A_1, B_1, C_1, D_1 \in \mathbb{C}^{n\times n}$ and $A_2, B_2, C_2, D_2 \in \mathbb{C}^{m\times m}$. Then the block direct sum $\oplus_b : \mathbb{C}^{2n\times 2n} \times \mathbb{C}^{2m\times 2m} \to \mathbb{C}^{2(n+m)\times 2(n+m)}$ is defined as*

$$\begin{bmatrix} A_1 & B_1 \\ C_1 & D_1 \end{bmatrix} \oplus_b \begin{bmatrix} A_2 & B_2 \\ C_2 & D_2 \end{bmatrix} = \begin{bmatrix} A_1 \oplus A_2 & B_1 \oplus B_2 \\ C_1 \oplus C_2 & D_1 \oplus D_2 \end{bmatrix}. \tag{36}$$

B Factorizing probabilities over block direct sums

Theorem 3 (Factorization of probabilities). *Consider a 1-mode POVM $\{R_i\}_{i\in I}$ for some index set $I = \{0, 1\}$ or $I = \mathbb{N}_0$, where R_i is either P_i or*

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Q_i described by Eq. (3) and Eq. (4). A d-mode Gaussian state with complex displacement vector γ and Q-function covariance matrix Σ. Suppose that the probability of detecting $S \in I^d$ is

$$\mathrm{tr}\left[\rho\left(P_{S_1} \otimes \ldots P_{S_d}\right)\right] = f\left(S, \mathrm{br}_S\, \gamma, \mathrm{br}_S\, \Sigma^{-1}\right) N(\gamma, \Sigma), \tag{37}$$

where the normalization N has the block matrix factorization property, i.e.

$$N(\gamma_1 \oplus_b \gamma_2, \Sigma_1 \oplus_b \Sigma_2) = N(\gamma_1, \Sigma_1) N(\gamma_2, \Sigma_2). \tag{38}$$

Then suppose ρ_1, ρ_2 are Gaussian states over d_1 and d_2 modes with γ_1 and γ_2 complex displacement vectors and Σ_1, Σ_2 Q-function covariance matrices respectively, and consider $S \in I^{d_1}$, $T \in I^{d_2}$. Then f also has the block matrix factorization property in the following sense:

$$\begin{aligned} &f(S \times T, \mathrm{br}_{S\times T}(\gamma_1 \oplus_b \gamma_2), \mathrm{br}_{S\times T}(\Sigma_1^{-1} \oplus_b \Sigma_2^{-1})) \\ &\qquad = f(S, \mathrm{br}_S\, \gamma_1, \mathrm{br}_S\, \Sigma_1^{-1}) f(T, \mathrm{br}_T\, \gamma_2, \mathrm{br}_T\, \Sigma_2^{-1}). \end{aligned} \tag{39}$$

Proof. By direct calculation,

$$\begin{aligned} &f(S \times T, \mathrm{br}_{S\times T}(\gamma_1 \oplus \gamma_2), \mathrm{br}_{S\times T}(\Sigma_1^{-1} \oplus \Sigma_2^{-1})) \\ &\qquad = \frac{\mathrm{tr}\left[(\rho_1 \otimes \rho_2)\left(P^{(S)} \otimes P^{(T)}\right)\right]}{N(\gamma_1 \oplus_b \gamma_2, \Sigma_1 \oplus_b \Sigma_2)} = \frac{\mathrm{tr}\left[\rho_1 P^{(S)}\right] \mathrm{tr}\left[\rho_2 P^{(T)}\right]}{N(\gamma_1, \Sigma_1) N(\gamma_2, \Sigma_2)} \\ &\qquad = f(S, \mathrm{br}_S\, \gamma_1, \mathrm{br}_S\, \Sigma_1^{-1}) f(T, \mathrm{br}_T\, \gamma_2, \mathrm{br}_T\, \Sigma_2^{-1}), \end{aligned} \tag{40}$$

where $P^{(V)} = P_{V_1} \otimes \cdots \otimes P_{V_d}$, for any $V \in I^d$. □

Corollary 1. *The torontonian, loop torontonian, hafnian and loop hafnian also factorize in the manner described by Theorem 3.*

C Supplementary calculations

Proposition 1. *Let $U \in U(d)$ and $D \in \mathbb{C}^{d\times d}$ diagonal matrix, and $S = 1^n 0^{(d-n)}$ with $n < d$. Then*

$$\mathrm{r}_S\left(UDU^\dagger\right) = \mathrm{rr}_S\left(U\right) D\, \mathrm{cr}_S\left(U^\dagger\right) =: VDV^\dagger, \tag{41}$$

where $V = \mathrm{rr}_S\left(U\right) \in \mathbb{C}^{n\times d}$, and rr, cr are defined in Appendix A.

Proposition 2. *Let $U \in U(d)$ be an m-bandwidth unitary, and let $m < n < d$, $S = 1^n 0^{(d-n)}$. Then let V be defined by*

$$\mathrm{rr}_S\left(U\right) =: V = \left[W \middle| X\right]. \tag{42}$$

where $W \in \mathbb{C}^{n\times(n-m)}$, $X \in \mathbb{C}^{n\times(d-n+m)}$. Then $V^\dagger V = \mathbb{1}_{n-m} \oplus K$, where $X^\dagger X = K \in \mathbb{C}^{(d-n+m)\times(d-n+m)}$.

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Proof. $U \in U(d)$ can be written using d unit vectors $\{\boldsymbol{u}_i\}_{i=1}^{d}, \boldsymbol{u}_i \in \mathbb{C}^d$ as $U = [\boldsymbol{u}_1, \dots \boldsymbol{u}_d]$, where $\langle \boldsymbol{u}_i, \boldsymbol{u}_j \rangle = \delta_{ij}$ and $\langle \cdot, \cdot \rangle$ is the standard inner product over $\mathbb{C}^d$. When we reduce by $S = 1^n 0^{d-n}$, elements from $\boldsymbol{u}_i$ are removed consequently. Split up the reduced matrix as $V = [W|X]$. We know that $W^\dagger W = \mathbb{1}_{n-m}$ since i, j fulfill the conditions $i, j \leq n - m$, and the reduction only removes zero elements from $\boldsymbol{u}_i$ and $\boldsymbol{u}_j$. More concretely, one can write $\mathrm{rr}_S \, \boldsymbol{u}_i = \boldsymbol{w}_i \oplus 0_{n-i-m}$ which is still orthogonal to $\boldsymbol{u}_j$ vectors where only zeros have been trimmed. Moreover, $W^\dagger X = 0$, since for $i \leq n - m$ and $j > n - m$, the reduction by S only cancels zeros from $\boldsymbol{u}_i$, and the non-zero elements cancelled in $\boldsymbol{u}_j$ by the reduction are multiplied by zero when calculating the inner product with $\boldsymbol{u}_i$, hence the inner product of reduced vectors is equal to the inner product of original vectors in this case. Putting everything together one can conclude that $V^\dagger V = \mathbb{1}_{n-m} \oplus X^\dagger X$. □

Proposition 3. *Let $U \in U(d)$ be a unitary and let $n \in [d]$, $S = 1^n 0^{d-n}$. Let $V = \mathrm{rr}_S(U)$ and $D \in \mathbb{C}^{d \times d}$ a diagonal matrix. Then*

$$(VDV^\dagger)^{-1} = VD^{-1}V^\dagger. \tag{43}$$

Proposition 4. *Let $\Sigma \in \mathbb{C}^{2d \times 2d}$ be a Q-function covariance matrix of the form*

$$\Sigma = \begin{bmatrix} U & \\ & U^* \end{bmatrix} \begin{bmatrix} \cosh^2 r & \cosh r \sinh r \\ \cosh r \sinh r & \cosh^2 r \end{bmatrix} \begin{bmatrix} U^\dagger & \\ & U^T \end{bmatrix}, \tag{44}$$

where $U \in U(d)$ is m-bandwidth, and $k := 2m$. Let $F = 1^n 0^{d-n}$ and $S = 1^{n-k} 0^k$ with $k \leq n \leq d$. Then

$$(\mathrm{br}_S \circ \mathrm{inv} \circ \mathrm{br}_F)\Sigma = \begin{bmatrix} \mathbb{1} & -\mathrm{r}_S \, \mathrm{r}_F(B) \\ -\mathrm{r}_S \, \mathrm{r}_F(B)^* & \mathbb{1} \end{bmatrix}. \tag{45}$$

where $B = U \tanh(r) U^T$.

Proof. Let us denote $\cosh^2(r) =: C$ and $\cosh(r)\sinh(r) =: S$. Then

$$\mathrm{br}_F \, \Sigma = \begin{bmatrix} VCV^\dagger & VSV^T \\ V^*SV^\dagger & V^*CV^T \end{bmatrix}, \tag{46}$$

using Proposition 1. The inverse can be divided into blocks as

$$(\mathrm{br}_F \, \Sigma)^{-1} = \begin{bmatrix} (\mathrm{br}_F \, \Sigma)^{-1}_{11} & (\mathrm{br}_F \, \Sigma)^{-1}_{12} \\ (\mathrm{br}_F \, \Sigma)^{-1}_{21} & (\mathrm{br}_F \, \Sigma)^{-1}_{22} \end{bmatrix}. \tag{47}$$

By explicit calculation, one can show that

$$(\mathrm{br}_F \, \Sigma)^{-1}_{11} = \left(V(C - SV^T(V^*CV^T)^{-1}V^*S)V^\dagger\right)^{-1}, \tag{48}$$

and using Proposition 3 we can write

$$C - SV^T(V^*CV^T)^{-1}V^*S = C - SV^TV^*C^{-1}V^TV^*S. \tag{49}$$

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Moreover, using Proposition 2 we may write

$$\begin{aligned} C - SV^T V^* C^{-1} V^T V^* S &= C - S(\mathbb{1}_{n-m} \oplus K^*) C^{-1} (\mathbb{1}_{n-m} \oplus K^*) S \\ &=: \mathbb{1}_{n-m} \oplus M, \end{aligned} \tag{50}$$

where $K, M \in \mathbb{C}^{(d+m-n)\times(d+m-n)}$. We also know that

$$\left(V(\mathbb{1} \oplus M)V^\dagger\right)_{ij} = \sum_{a,b=1}^{d} V_{ia} (\mathbb{1}_{n-m} \oplus M)_{a,b} V^*_{jb}, \tag{51}$$

but since V is m-bandwidth, we know that there is no terms overlapping with m if $i, j \leq n-m-m = n-k$. Therefore it is guaranteed that $(\mathrm{br}_F\, \Sigma)^{-1}_{11} = \mathbb{1}_{n-k} \oplus E$, where $E \in \mathbb{C}^{(d+k-n)\times(d+k-n)}$, which means that $\mathrm{r}_S(\mathrm{br}_F\, \Sigma)^{-1}_{11} = \mathbb{1}_{n-k}$. Similarly, one can write

$$(\mathrm{br}_F\, \Sigma)^{-1}_{12} = -(\mathbb{1}_{n-k} \oplus E)\; VSV^T V^* C^{-1} V^T, \tag{52}$$

and after reduction one acquires

$$\mathrm{r}_S((\mathrm{br}_F\, \Sigma)^{-1}_{12}) = -\,\mathrm{r}_S\left(V(\mathrm{r}_G(\tanh r) \oplus H)V^T\right), \tag{53}$$

where $G = 1^{(n-m)}0^{(d-n+m)}$ and $H \in \mathbb{C}^{(d+m-n)\times(d+m-n)}$. Consider indices $i, j \leq n-k$. Then

$$\left(V(\mathrm{r}_G(\tanh(r)) \oplus H)V^T\right)_{ij} = -\sum_{a,b=1}^{d} V_{ia} \left(\mathrm{r}_G(\tanh(r)) \oplus H\right)_{ab} V_{bj}, \tag{54}$$

but we know that $V_{ia} = V_{bj} = 0$ for $a, b > n-m$, i.e. the values of H are irrelevant when we are computing matrix elements with indices $i, j \leq n-k$. Therefore we can just write

$$\left(V(\mathrm{r}_G(\tanh(r)) \oplus H)V^T\right)_{ij} = \left(V \tanh(r) V^T\right)_{ij}, \tag{55}$$

which essentially yields that

$$\begin{aligned} \mathrm{r}_S(\mathrm{br}_F(\Sigma)^{-1})_{12} = -\,\mathrm{r}_S\,\mathrm{r}_F(V \tanh(r) V^T) &= -\,\mathrm{r}_S\,\mathrm{r}_F(U \tanh(r) U^T) \\ &= -\,\mathrm{r}_S\,\mathrm{r}_F(B). \end{aligned} \tag{56}$$

□

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