Eur. Phys. J. Plus (2026) 141:368
https://doi.org/10.1140/epjp/s13360-026-07590-z

THE EUROPEAN PHYSICAL JOURNAL PLUS

Regular Article

Leveraging qudits: high-dimensional Grover adaptive search algorithm for solving quadratic and higher-order unconstrained binary optimization problems

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Received: 16 January 2026 / Accepted: 17 March 2026
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Abstract The Grover Adaptive Search (GAS) is an innovative approach offering solutions to optimization problems thanks to quadratic speedup enabled by the Grover Search Algorithm. However, the need for more qubits, depending on the number of variables in optimization problems, creates problems in providing optimal solutions. The central premise of this study is the principle that d-dimension is more efficient than 2-dimension could lead to more advantageous results when the GAS algorithm is adapted to d-dimension. To that end, this study adapts the GAS algorithm to the d-dimension drawing on quantum computing in the d-dimension, allowing computing using fewer quantum resources, namely, qudits. The proposed algorithm is validated against the Quadratic and Higher-Order Unconstrained Binary Optimization (QUBO-HUBO). This study concludes the d-dimensional GAS algorithm achieves solutions using fewer qudits for these problems in the QUBO and the HUBO. This study underscores the progress achieved in the advancement of high-dimensional quantum computing.

1 Introduction

The quantum computing paradigm is advantageous in computational science thanks to the superior features like superposition and entanglement provided by quantum mechanics. These advantages are clearly present in algorithms such as Shor's factorization algorithm [1] and Grover Search (GS) algorithm [2]. GS [2] algorithm is a search algorithm that intends to find the desired value in an unsorted database, achieving a quadratic speedup in comparison to its classical counterparts [2].

Grover Adaptive Search [3] (GAS) algorithm is an algorithm that aims to find the solution of optimization problems such as the Quadratic Unconstrained Binary Optimization (QUBO) and Higher-Order Unconstrained Binary Optimization (HUBO) using the GS [2] algorithm. This algorithm is based on two main constructs: i- Quantum Dictionary [4] (QD), which represents encoding optimization problems and inspired by the concept of dictionary, which creates key-value pairs commonly used in classical computer science, and ii- the GS [2] algorithm which uses an iterative approach in GAS [3] algorithm.

QUBO [5] is a widely used mathematical modeling to solve optimization problems through quantum computing. Yet, the growing number of inputs in problems and the subsequent increase in variables, along with the necessity for qubits representing these variables in quantum form, pose challenges in achieving efficient solutions due to existing limitations in quantum technology. Therefore, previous research has focused on reducing the number of variables using different encoding techniques and, consequently, reducing the need for qubits [6, 7]. Various encoding techniques result in problems being expressed with higher-order terms, which in turn lead to additional variable costs [8] for seeking solutions through methods such as quantum annealing (QA) [9]. Since quantum annealing provides solutions to optimization problems in the QUBO (specifically, the problems with the highest order degree being 2). Hence, the significance of the GAS algorithm lies in the fact that it can provide solutions to both problems in the QUBO and higher-order terms.

Indeed, the importance of the GAS algorithm is underscored by the fact that numerous optimization problems [10–13] also rely on it to search for solutions. Besides its application to optimization problems, scholarly efforts have been underway to enhance the efficiency of the GAS algorithm. For example, Sano et al. [14] propose two new strategies for higher-order binary formulations. The first strategy decreases the number of gates by polynomial factorization, while the other reduces the order of the objective function by half. Moreover, using their high-order strategies, they achieved a reduction in the number of qubits used relative to the number of qubits used in the original QUBO function. As a result, circuit runtime and implementation cost are decreased. Further, Norimito et al. [15] proposed a quantum algorithm that solves Higher-Order Unconstrained Binary Optimization (HUBO) problems with integer coefficients and supports real-valued HUBO problems, inspired by GAS. The studies mentioned here is performed using the

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Published online: 02 April 2026

GAS algorithm in 2-dimensional. To our knowledge, there is no research using higher-dimensional quantum computing for GAS algorithm.

Quantum computing typically involves a two-level system using ground and excited states. These two-level systems are specifically called quantum bits (qubits). Higher-dimensional quantum computing, on the other hand, offers a structure with an extra level where information can be used [16]. Structures with this extra level (where $d > 2$ [17]) are called quantum digits or qudits for short. This additional level provides the following advantage when encoding information: to represent an N-dimensional system in terms of qubits, we need at least $log_2 N$ qubits, while to describe it in terms of qubits, we need $log_d N$ qudits [18]. This extra level also offers advantages over two-level computation in terms of a larger search space and, consequently, lower circuit complexity [18–21], noise resistance [22]. In addition, the advantages of quantum gate diversity and the wealth of entanglement structures [16] are motivating results for studying quantum computation in higher dimensions. As a result, it has been proven that computations can be carried out with fewer quantum resources using the d-dimensional version of the GS algorithm for multiple targets [23]. Here, it is particularly important to note that the GAS algorithm and the GS algorithm are distinct algorithms, complementing each other but serving different purposes. The potential advantages of high dimensionality mentioned above have also begun to be used in machine learning [16] and optimization problem solving [24, 25]. Thus, the use of high-dimensional quantum computation to solve optimization problems [24, 25] demonstrates that we are rapidly advancing to a stage where high-dimensional quantum computing can serve as a solution to optimization problems, and its potential deserves more comprehensive exploration. Therefore, the potential advantages of the GAS algorithm for optimization problems in higher dimensions should be investigated.

Each variable constituting the optimization problem in the 2-dimensional GAS algorithm is mapped to 1 qubit. This leads to the use of an excessive number of qubits even when creating the input data of the problem. The number of qubits required in the 2-dimensional GAS algorithm increases when the output qubit cost is added. Therefore, the problem of storing and processing information is a major challenge for the GAS algorithm. The aim of this study is twofold: first, to investigate whether the GAS algorithm can be implemented in high dimensions; and second, if so, to demonstrate the potential advantage of d-dimensional quantum computing in overcoming the aforementioned shortcomings of GAS. To illustrate this advantage, optimization problems in the QUBO [3] and HUBO [14] formats, which can be solved by quantum computing, are used. In this regard, the results obtained when compared with the 2-dimensional GAS algorithm show that the information storage capability provided by high dimensionality is also preserved in the HD-GAS algorithm, can be used to solve optimization problems and provides a logarithmic advantage. All implementations in this study are performed using the Cirq [26] quantum simulator, which can perform high-dimensional quantum computing.

This study is outlined as follows: Sect. 2 offers the proposed high-dimensional GAS algorithm. Section 3 concludes with the implementation of HD-GAS algorithm for different examples. Section 4 includes results and discussion. Lastly, some remarks are offered in Sect. 5.

2 Constructing High-Dimensional Grover Adaptive Search (HD-GAS) algorithm

The proposed high-dimensional GAS algorithm expresses the key, value pairs that form the basis of the GAS algorithm drawing on qudits, which serve to store more information using fewer quantum resources. After the key and value pairs are encoded into qudits, the state preparation operator is introduced in equal superposition. This defines the A_y^d operator. The mathematical form of this expression is presented in Eq. (2). Then, this operator is fed to the d-dimensional GS algorithm to create the HD-GAS algorithm, where the d-dimensional GS algorithm is constructed similar to the study of Acar et al. [23]. The mathematical equations required for the HD-GAS algorithm are presented below:

$$|\psi\rangle = |0_d\rangle_n |0_d\rangle_m \tag{1}$$

$$A_y^d |0_d\rangle_n |0_d\rangle_m = \frac{1}{\sqrt{d^n}} \sum_{c=0}^{d^n-1} |c\rangle_n |g(c) - y\rangle_m. \tag{2}$$

Where n-qudit is the input register and m-qudit is the output register, all $|c\rangle|g(c)-y\rangle_m$ outputs are prepared in the equal superposition state in the form of key-value pair as follows [27].

The Grover operator in the d-dimension is expressed as follows [27]:

$$G_d = A_{y_j}^d D^d (A_{y_j}^d)^\dagger O^d. \tag{3}$$

where O^d is the d-dimensional oracle operator acting on a single qubit, D^d is the d-dimensional Grover diffusion operator and $(A_{y_j}^d)^\dagger$ is the hermitian of the operator $A_{y_j}^d$.

Algorithm 1 Proposed HD-GAS [27]

Input: g: $X \in Z$, $\lambda = 8/7$.
Uniformly sample $c_1 \in X$ and set $y_1 = g(c_1)$.
Set $t = 1$, $j = 0$.
repeat
  Randomly select the rotation count L_j from the set $\{0, 1, \ldots, \lceil t-1 \rceil\}$.
  Implement **High-Dimensional GS** with L_j iterations, using $\mathbf{A^d_{y_j}}$ and $\mathbf{O^d_{y_j}}$. The outcomes of this measurement are the outputs c and y respectively.
  if $y < y_j$ **then**
    $c_{j+1} = c$, $y_{j+1} = y$, and $t = 1$
  else
    $c_{j+1} = c$, $y_{j+1} = y$, and $t = min\{\lambda t, \sqrt{2^n}\}$
  j=$j+1$
until *a termination condition is met*;

Algorithm 1 presents the pseudocode generated for the HD-GAS algorithm [27], i.e., for qudit systems, using the equations above.

3 Solving QUBO and HUBO problems using HD-GAS algorithm

This section begins with a brief introduction to QUBO and HUBO problems. It, then, presents steps for creating the HD-GAS algorithm as well as the results of measurement. It is worth noting that the number of variables is crucial for the decision regarding the dimension to be used in quantum computing. This study encodes 3 input (key) variables in the discussed problems with a single qudit in the 8 dimension. Although this study concentrates on $d = 8$, it can also be extended to any dimensions of d.

The mathematical models commonly used for solving optimization problems with quantum computing are QUBO and HUBO. The QUBO model terms of a maximum of degree 2, while the HUBO model consists of terms of order 3, 4 or higher. Below is the mathematical form of the QUBO model.

$$\text{min/max} \sum_i Q_{ii} + \sum_{i<j} Q_{ij} \tag{4}$$

where Q is the upper triangular or symmetric matrix and x is the binary decision variable [5].

3.1 Illustrative example for solving QUBO using HD-GAS

Gilliam et al. [3] modeled a portfolio optimization problem in the QUBO. This model is as follows:

$$-x_0 + 2x_1 - 3x_2 - 2x_0x_2 - x_1x_2. \tag{5}$$

For this example, the HD-GAS algorithm is created as follows. This problem can be solved in the 8 dimension using the proposed HD-GAS algorithm with 1 input qudit, 2 output qudits, and 1 ancilla qudit.

Step 1

With input qudit being $n = 1$, output qudits $m = 2$ and $d = 8$, the quantum state is initialized as follows:

$$|\psi\rangle = |0_8\rangle_1 |0_8\rangle_2$$

Then, the Hadamard (H_8) operator is applied to the input and output qudits, thus providing equal-amplitude superposition for higher dimensions.

$$H_8^{\otimes 3} |\psi\rangle = \left(\frac{1}{\sqrt{8}}\right)^3 \sum_{i=0}^{7} \sum_{j=0}^{7} |i\rangle_1 |j\rangle_2$$

Step 2

Creating a quantum dictionary requires high-dimensional controlled phase gates. The mathematical definition of this gate and its circuit representation for an example are presented below:

$$C_8^L ({}_{k,r}P_d^p) |i\rangle_1 |j\rangle_2 = |i\rangle ({}_{k,r}P_d^p)^{\prod_{l \in L} i_l} |j\rangle_2$$

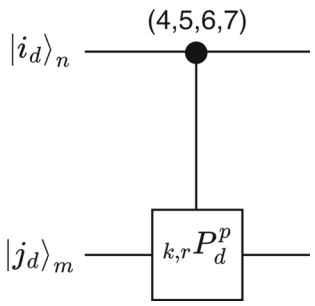


Fig. 1 High dimension controlled Phase gate

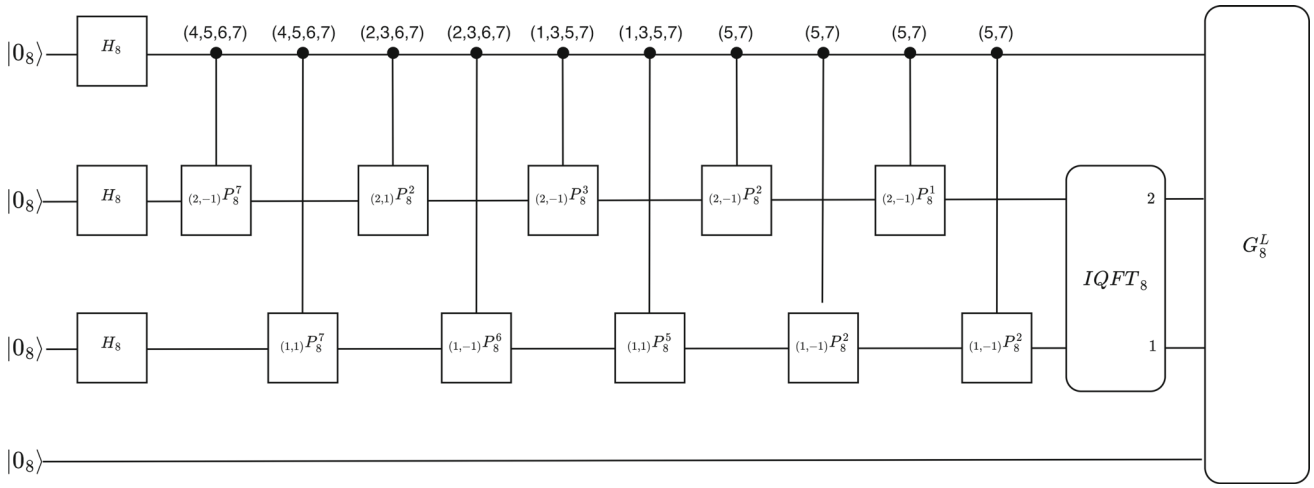


Fig. 2 where $A_{y\,j=0}^d$, $-x_0 + 2x_1 - 3x_2 - 2x_0x_2 - x_1x_2$ quantum circuit in high dimension with 1 key qudit, 2 value qudits, and 1 ancilla qudit [27]

The representation of the controlled gate in a quantum circuit in high dimension, whose mathematical expression is given above, is as follows: The quantum gate corresponding to controlling the states 4, 5, 6, 7 in a quantum state of 8 dimensions, where $L = \{4, 5, 6, 7\}$, is presented in Fig. 1.

In here, H_8 and $_{k,r}P_d^p$ are higher-dimensional quantum gates [18, 28]. Also k = root, r = rotation, p = power of matrices.

$$ {}_{k,r}P_d^p = \begin{bmatrix} w^0 & 0 & 0 & 0 & \dots & 0 \\ 0 & w^1 & 0 & 0 & \dots & 0 \\ \vdots & 0 & w^2 & 0 & \dots & \vdots \\ 0 & 0 & 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & 0 & \dots & w^{d-1} \end{bmatrix} $$

where $w = e^{2\pi irp/d^k}$.

Step 3

In this step, a high-dimensional Inverse Quantum Fourier Transform (*IQFT*) is applied to the output qudits of the created quantum circuit. The goal is to end in an encoded state as a superposition of key-value pairs. This corresponds to the expression in Eq.(2).

Step 4

The high-dimensional diffusion, oracle, and Hermitian of the operator A_y^d required for high-dimensional Grover iteration are generated, which correspond to the operations in Eq. (3). Then, the resulting Grover iterative operator and the process shown in the pseudocode in Algorithm 1 are applied. These operations produce the outcome of the optimization problem.

Figure 2 shows the high-dimensional quantum circuit resulting from the application of these four steps for Illustrative Example 1.

Figure 3 offers the results obtained on running the quantum circuit in Fig. 2 on Cirq 1000 times. These results demonstrate that the HD-GAS algorithm obtains -6, which is the lowest value with a probability of 98.4%.

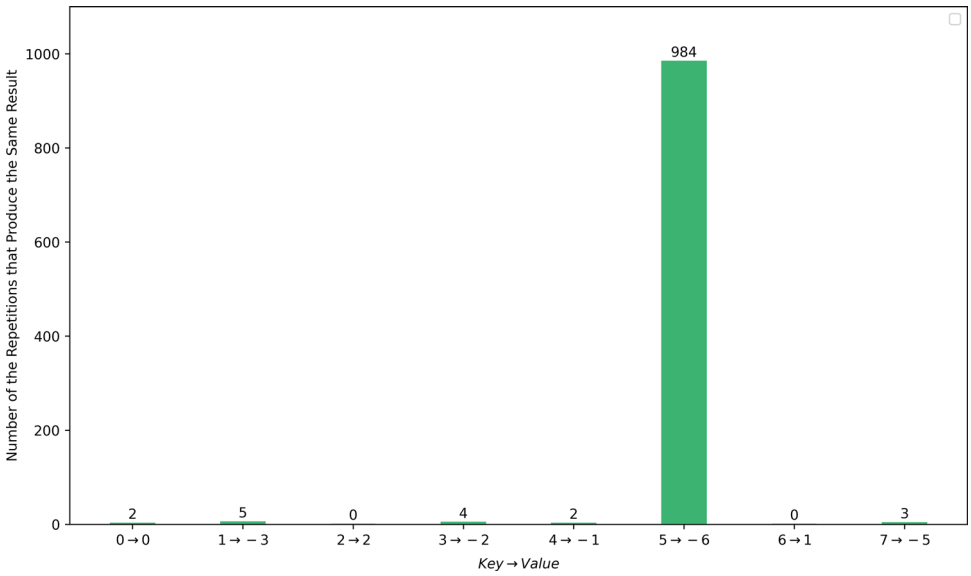


Fig. 3 Results obtained on running the quantum circuit in Fig. 1 on Cirq for 1000 times [27]

3.2 Illustrative example for solving HUBO using HD-GAS algorithm

Sano et al. [14] studied the solution of $x_1x_2x_3 + x_1x_3 - x_3$, which is a HUBO-ASC/DSC problem drawing on the GAS algorithm (Kindly see Sano et al's work for more information on HUBO formulations with ascending/descending assignment). This problem is solved using the proposed HD-GAS algorithm method in 8 dimensions with 1 input qudit, 1 output qudit, and 1 ancilla qudit. For this example, the HD-GAS algorithm is created as follows.

Step 1

For this example input qudit $n = 1$, output qudit $m = 1$ and $d = 8$, the quantum state is initialized as follows:

$$|\psi\rangle = |0_8\rangle_1|0_8\rangle_1$$

Then, the Hadamard (H_8) operator is applied to both the input and output qudits, thereby providing an equal-amplitude superposition for higher dimensions.

$$H_8^{\otimes 2}|\psi\rangle = \left(\frac{1}{\sqrt{8}}\right)^2 \sum_{i=0}^{7}\sum_{j=0}^{7}|i\rangle_1|j\rangle_1$$

Step 2

Problem-specific controlled phase gates are created for the quantum dictionary.

$$C_8^L({}_{k,r}P_d^p)|i\rangle_1|j\rangle_1 = |i\rangle({}_{k,r}P_d^p)^{\prod_{l\in L} i_l}|j\rangle_1$$

Step 3

In this step, the Inverse Quantum Fourier Transform (*IQFT*) is applied to the output qudit of the circuit created. However, applying *IQFT* to a single qudit corresponds to the $H_8^\dagger$ gate. Therefore, the $H_8^\dagger$ gate is applied to the output qudit. The goal is to end the encoded state in a superposition of key-value pairs. This corresponds to the expression in Eq. (2).

Step 4

The high-dimensional diffusion, oracle, and Hermitian of the operator A_y^d required for high-dimensional Grover iteration are generated, which correspond to the operations in Eq. (3). Then, the resulting Grover iterative operator and the process shown in the pseudocode in Algorithm 1 are applied. These operations produce the outcome of the optimization problem.

Figure 4 shows the high-dimensional quantum circuit resulting from the application of these four steps for Illustrative Example 2:

The quantum circuit ${A_y^d}_{j=0}$ in Fig. 4, which is necessary for the solution of this problem, can be established through Eq. (2).

Figure 5 offers the results from running the quantum circuit in Fig. 4 on Cirq 1000 times. These results indicate that the HD-GAS algorithm obtains the lowest value, -1, with a total probability of 98.6% for two different input values.

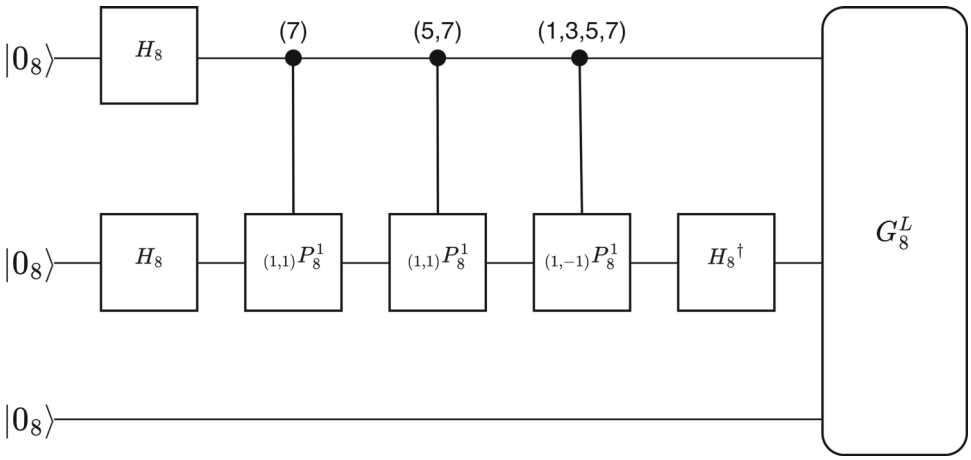


Fig. 4 where $A^d_{y\,j=0}$, $x_1x_2x_3 + x_1x_3 - x_3$ quantum circuit in high dimension with 1 key qudit, 1 value qudit, and 1 ancilla qudit [27]

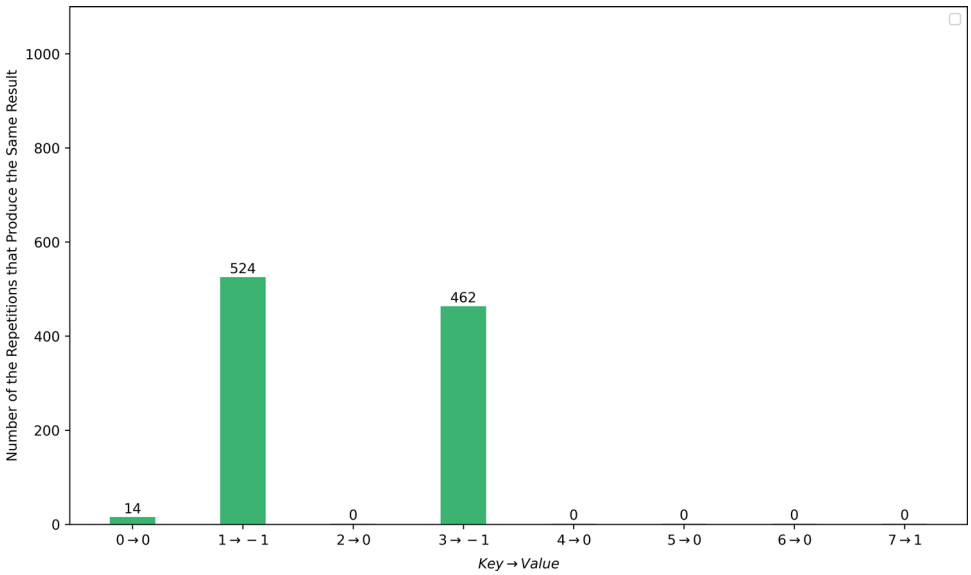


Fig. 5 Results obtained on running the quantum circuit in Fig. 4 on Cirq 1000 times [27]

3.3 Illustrative example for solving HUBO-PF using HD-GAS algorithm

Sano et al. [14] factorized the HUBO-ASC/DSC function above into $x_1x_2x_3 - (1 - x_1)x_3$, which they called the HUBO-PF method. In doing so, they decreased the number of quantum gates required for the GAS algorithm. The use of the HUBO-PF method with the HD-GAS algorithm, results in both fewer quantum resources in the high dimension, and a decreased number of gates used in the high dimension, as shown in the study of Sano et al. [14].

Step 1

For this example input qudit $n = 1$, output qudit $m = 1$ and $d = 8$, the quantum state is initialized as follows:

$$|\psi\rangle = |0_8\rangle_1|0_8\rangle_1$$

Then, the Hadamard (H_8) operator is applied to both the input and output qudits, thereby providing an equal-amplitude superposition for higher dimensions.

$$H_8^{\otimes 2}|\psi\rangle = \left(\frac{1}{\sqrt{8}}\right)^2 \sum_{i=0}^{7}\sum_{j=0}^{7}|i\rangle_1|j\rangle_1$$

Step 2

Problem-specific controlled phase gates are created for the quantum dictionary.

$$C_8^L({}_{k,r}P_d^p)|i\rangle_1|j\rangle_1 = |i\rangle({}_{k,r}P_d^p)^{\prod_{l\in L} i_l}|j\rangle_1$$

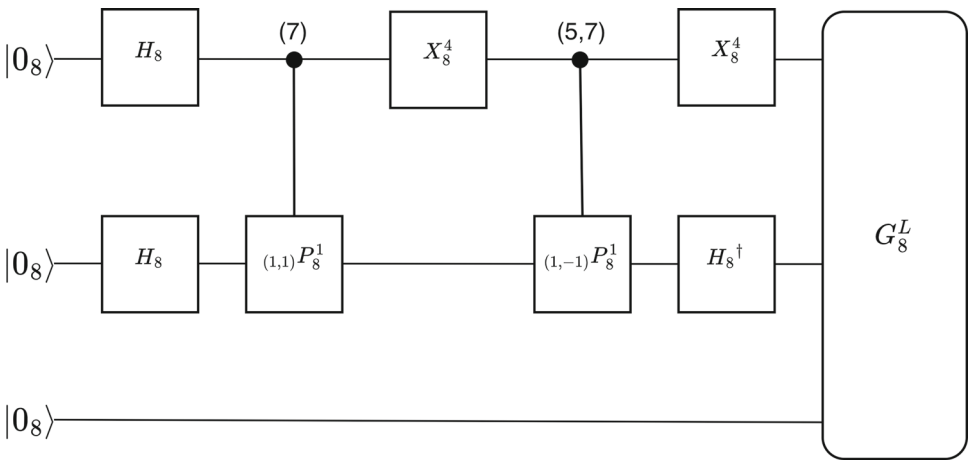


Fig. 6 where $A_{y\,j=0}^d$, $x_1x_2x_3 - (1-x_1)x_3$ quantum circuit in high dimension with 1 key qudit, 1 value qudits, and 1 ancilla qudit [27]

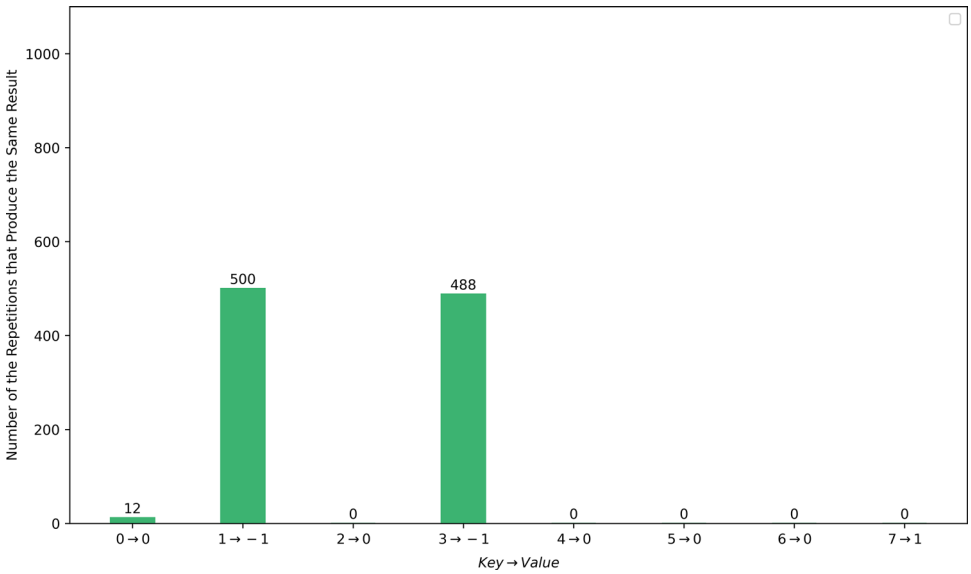


Fig. 7 Results obtained on running the quantum circuit in Fig. 6 on Cirq for 1000 times [27]

Step 3

In this step, a high-dimensional Inverse Quantum Fourier Transform (*IQFT*) is applied to the output qudit of the created quantum circuit. However, applying *IQFT* to a single qudit corresponds to the $H_8^\dagger$ gate. Therefore, the $H_8^\dagger$ gate is applied to the output qudit. The goal is to end the encoded state in a superposition of key-value pairs. This corresponds to the expression in Eq.(2).

Step 4

The high-dimensional diffusion, oracle, and Hermitian of the operator A_y^d required for high-dimensional Grover iteration are generated, which correspond to the operations in Eq. (3). Then, the resulting Grover iterative operator and the process shown in the pseudocode in Algorithm 1 are applied. These operations produce the outcome of the optimization problem.

Figure 6 shows the high-dimensional quantum circuit resulting from the application of these four steps for Illustrative Example 3.

In the quantum circuit in Fig. 6, X_8^4 is higher-dimensional quantum gate [29].

Figure 7 offers the results from running the quantum circuit in Fig. 6 on Cirq 1000 times. These results indicate that the HD-GAS algorithm obtains the lowest value, -1, with a total probability of 98.8% for two different input values.

4 Results and discussion

This section compares the number of qubits and qudits respectively used in the GAS and HD-GAS algorithms for the studied problems. Table 1 presents the required quantum resource (qubit-qudit) numbers in 2-dimensional and higher dimensions for the QUBO and HUBO problems in Sect. 3. Though the number of variables in these problems is low, the GAS algorithm in the d-dimension is advantageous in terms of the number of qudits required. While the total number of input and output qubits with ancilla is represented as $n+m+1$ in the 2-dimensional GAS algorithm, the total number of qudits in the proposed HD-GAS algorithm is as

Table 1 Comparison of the GAS and HD-GAS Algorithms

	GAS				Proposed HD-GAS [27]			
	Input Qubit	Output Qubit	Ancilla	Total Qubit	Input Qudit	Output Qudit	Ancilla	Total Qudit
QUBO [30]	3	6	1	10	1	2	1	4
HUBO [14]	3	3	-	6	1	1	1	3
HUBO-PF [14]	3	3	-	6	1	1	1	3

follows: $log_d(2^n) + log_d(2^m) + 1$. This indicates clearly that the HD-GAS algorithm allows the solution of optimization problems using fewer qudits.

To summarize, the performance of the proposed HD-GAS algorithm has been tested against different optimization problems, one in the QUBO and the other in the HUBO [3, 14]. Given the capacity of the HD-GAS algorithm to solve HUBO problems, reducing the problems in this study to QUBO to solve them would require additional variables and creating a penalty coefficient [8]. Therefore, it is likely that this will also increase the quantum resources to be used. For this reason, this method was not preferred.

Based on the results, the HD-GAS algorithm is advantageous in problems even with very few variables in terms of the number of quantum resources relative to the GAS algorithm. Considering the number of variables in real-world problems, it is evident that high-dimensional quantum computing will provide efficient solutions. In addition, the HD-GAS algorithm is applied to find the minimum value of the function obtained by the HUBO-PF [14] method. As a result, there is a decrease in the number of quantum resources used in the HD-GAS algorithm, which can be seen in the quantum circuit in Fig. 6.

Lastly, performing quantum computing on circuit-based qudit systems presents implementation challenges compared to qubit systems [23], and quantum simulators similar to those for qubit systems are not currently available. Also, studies on qudit systems are largely confined to theoretical or experimental settings. One such experimental study is the implementation of the Grover Search Algorithm on qudit systems using the ion trapping method [31]. Since the Grover Search Algorithm is a crucial component of the proposed HD-GAS algorithm, it has the potential to be implemented on qudit systems using the ion trapping method.

There are further experimental studies on qudit systems with Rydberg atoms, and since experimentally motivated research on the QAOA algorithm has been conducted on qudit systems, the HD-GAS algorithm also has the potential to be experimentally implemented with Rydberg atoms for qudit systems [32]. Moreover, a photon-based study implements the VQE algorithm experimentally on qudit systems [33]. The proposed HD-GAS algorithm has the potential to be executed also through photon-based quantum technologies. Since these experimental studies are at the experimental level, we implemented the proposed HD-GAS algorithm on the Cirq [26] quantum simulator, which enables quantum computing on qudit systems.

5 Conclusion

Using quantum computing to solve optimization problems enhances the efficiency of quantum computing in computational science. Optimization problems incorporate multiple variable and the number of qubits required for these variables is too many, which is problematic for current quantum computing technologies.

This study has attempted to search for solutions to different optimization problems expressed in the QUBO and HUBO through the proposed HD-GAS algorithm. Thus, the key and value pairs that enable the optimization problem in the GAS algorithm to form a QD are expressed in d-dimension, which allows the use of fewer quantum resources. The proposed method has been tested on the Cirq quantum computing simulator for different problems, one in the QUBO and the other in the HUBO. The results show that the number of quantum resources required to encode key and value pairs can be reduced. It should be noted that this study does not attempt to compare the number of quantum gates used in higher dimensions and the number of gates used in 2 dimensions.

This study concludes that the proposed HD-GAS algorithm successfully runs on qudit systems and that this would offer a solution to address the challenges with the capacity of qubits in optimization problems. Last but not the least, the proposed HD-GAS algorithm would potentially solve the optimization problems with real coefficients. To contribute positively to the future of high-dimensional quantum computing, it is considered crucial to examine how this work impacts real-world problems in the future. Overall, the significance of this study lies in the fact that the proposed HD-GAS algorithm holds a dual potential for both past and future studies that seek to solve optimization problems and also to use fewer qudits, as this algorithm is applicable to past studies to further decrease the number of qudits used and to future studies to help them decrease this number. Lastly, this study provides useful insights for experimental studies related to high dimension.

Acknowledgements This study has been produced as part of the doctoral dissertation of first author. Also, we sincerely appreciate the referee(s)' time in providing constructive feedback and valuable comments and suggestions, which helped greatly, improve the quality of our paper.

Funding Open access funding provided by the Scientific and Technological Research Council of Türkiye (TUBITAK). The authors thank TUBITAK ULAKBIM for supporting open access funding through the Springer Nature Read & Publish Agreement. The authors received no other specific funding for this study.

Data availability The code used in this study is available on GitHub: https://github.com/sabrigunduz/HD-GAS-Algorithm. The manuscript has associated data in a data repository.

Declarations

Conflict of interest The authors declare that they have no conflict of interest.

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