Solving complex problems of mixed-binary bounded optimization based on quantum algorithms

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ABSTRACT

The paper considers the ADMM (Alternating Direction Method of Multipliers) optimizer, which is a powerful tool for solving complex optimization problems, especially in the context of mixed-binary constrained optimization (MBCO). This study presents a new ADMM optimizer that demonstrates efficiency in solving optimization problems in the field of energy. The developed ADMM optimizer represents an innovative approach to solving optimization problems in the field of energy using quantum computing. It allows you to effectively solve MBCO tasks, taking into account various constraints and requirements related to energy production and distribution. The results of the study demonstrate the excellent performance and accuracy of the ADMM optimizer in comparison with other optimization methods. The developed ADMM optimizer represents a significant contribution to the field of optimization in the energy industry and has the potential for wide application in solving various tasks related to energy production and management.

Keywords: optimization, ADMM, mixed-binary optimization, energy, quantum computing, efficiency, environmental sustainability, application, optimization methods

1. INTRODUCTION

Optimization plays a key role in improving efficiency and optimizing processes in various industries, including logistics, finance, operations and energy. One of the most common classes of optimization problems are mixed-binary constrained optimization (MBCO) problems, which are found in various applied fields and represent complex problems requiring effective algorithmic methods to solve them [1-3]. In recent years, the variable direction multiplier method (ADMM) has become widely used as an effective method for solving optimization problems with constraints. ADMM is an iterative operator separation algorithm that can efficiently work with large amounts of data and complex constraints, ensuring convergence to an optimal solution [4-7]. This study presents a new ADMM optimizer specifically designed to solve optimization problems in the field of energy using quantum computing. The energy industry is facing a number of challenges, such as the need to maximize resource efficiency, reduce greenhouse gas emissions and increase the share of renewable energy sources. The introduction of quantum computing opens up new perspectives for solving these complex optimization problems. The purpose of this study is to present an ADMM optimizer capable of effectively solving MBCO tasks in the field of energy using quantum computing [8-11]. Mixed binary optimization (MBO) is a well-studied field within mathematical programming due to its wide range of applications in various fields. She is engaged in solving optimization problems that include both continuous and discrete variables, often characterized by the presence of integer variables. It is known that MBO is generally an NP-hard problem, which creates significant difficulties for exact solution methods [11-14].

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Third International Conference on Digital Technologies, Optics, and Materials Science (DTIEE 2024),
edited by Khamza Eshankulov, Arthur Gibadullin, Proc. of SPIE Vol. 13217, 1321712

English: Over the years, customizable solution methods, both precise and heuristic, have been developed in classical computing to solve the complexities associated with MBO formulations. These approaches differ depending on the specific structure and characteristics of the optimization task. With the advent of universal quantum computing, there has been increased interest in exploring the potential benefits of using quantum computing methods to solve combinatorial optimization problems such as MBO. Quantum variational approaches stand out especially in this context. These approaches involve parameterizing the quantum state space using a small set of parameters, and then optimizing these parameters using classical optimization methods to minimize or maximize the utility function [15-18]. This utility function is often represented by a Hamiltonian, which encodes the total energy of the system, which needs to be minimized. The variational theorem guarantees that the expected value of the Hamiltonian is greater than or equal to the minimum eigenvalue of the Hamiltonian [19-22].

Quantum variational approaches have found applications in various fields, including chemistry, machine learning, and mathematical optimization. In the context of mathematical optimization, special attention is paid to quadratic Unconstrained Binary Optimization (QUBO), where the goal is to minimize the quadratic function of binary variables [23-26]. The paper considers the application of the developed optimizer to solve specific problems in the energy industry, and also compares its performance with other optimization methods. The results obtained demonstrate the potential of the developed optimizer for solving complex optimization problems in the energy industry using quantum computing.

2. MATERIALS AND METHODS

This study uses the ADMM (Alternating Direction Method of Multipliers) optimizer, specially adapted to solve optimization problems.

The ADMM optimizer is an optimization method designed to solve convex optimization problems with constraints. It is especially effective for tasks that can be divided into subtasks or have a structure that allows you to separate variables.

Objective function and limitations:

Minimize:

$$f(x,u)=\sum_{i=1}^{n} f_i(x_i)=q(x)+\varphi(u), \tag{1}$$

With restrictions in general

With restrictions in general $Ax=b$ and $x \geq 0$,

Where A - the matrix, b - vector representing constraints or $Gx=b$, $g(x) \leq b$, $l(x,u) \leq 0$ and $x \geq 0$.

Here x - vector of variables, $f(x)$ - the target function.

Function $q: R^n \to R$ is quadratic, i.e.. $q(x)=x^T Qx + a^T x$ for a given symmetric square matrix $Q \in R^n \times R^n$, $Q=Q^T$ and the vector $a \in R^n$;

Set $\mathrm{X}=\{0,1\}^n=\{x_{(i)}(1-x_{(i)})=0,\ \forall i\}$ enforces binary restrictions;

The matrix $G \in R^n \times R^{n'}$, vector $b \in R^{n'}$ and the function $g: R^n \to R$ is convex;

Function $\varphi: R^l \to R$ is convex and U — convex set;

Function $l: R^n \to R^l$ is jointly convex in x,u.

If the original task is not in a form compatible with ADMM, it can be transformed. For example, constraints can be included in the target function using the Lagrange method.

ADMM is an iterative operator separation algorithm that uses the Lagrange multiplier method to solve problems with constraints. For the effective implementation of the ADMM algorithm in the context of energy tasks, appropriate adaptations and optimizations were carried out. To apply ADMM to MBCO, it is necessary to express the task in a standard form compatible with the ADMM method. This may require some transformations, such as approximating binary variables or formulating constraints in a specific form. The basic algorithm of the ADMM optimizer for solving convex optimization problems with constraints.

Step 1 - Initialization: Selection of initial values of variables x^0, Lagrange multipliers z^0, and auxiliary variables u^0. Usually the initial values are chosen randomly

Step 2 - Repeat:

2.1. Optimization x: Updating variables by minimizing the function:

$$x^{k+1} = \arg\min_x \left[f(x) + \frac{\rho}{2} \left\| Ax - b + z^k \right\|_2^2 \right] \tag{2}$$

2.2. Optimization z: Updating Lagrange multipliers z using updated variables x:

$$z^{k+1} = \arg\min_z \left[\frac{\rho}{2} \left\| Ax^{k+1} - b + z^k \right\|_2^2 \right] \tag{3}$$

Expression $\|v\|_2^2$ for the vector v It is usually defined as the sum of the squares of its components:

$$\|v\|_2^2 = \sum_{i=1}^{n} v_i^2 \tag{4}$$

Where v_i - i - melting the component of the vector v.

2.3. Updating Multipliers: Update auxiliary variables using updated variables x and z:

$$u^{k+1} = u^k + Ax^{k+1} - b + z^{k+1} \tag{5}$$

Updating the parameter ρ: Optional, but sometimes it is useful to change the parameter ρ, to ensure faster convergence. Usually ρ increase if the restrictions are not satisfied, and decrease otherwise.

Step 3. Quantum computing is used to solve optimization problems in the field of energy.

This study uses quantum optimization algorithms, QAOA (Quantum Approximate Optimization Algorithm), to solve the quantum optimization subtask that is included in the ADMM optimization process.

3.1. Setting the initial parameters of the algorithm, such as the depth of the quantum chain and the initial values of the angles γ and β.

3.2. Creation of the initial quantum state $|\psi(\gamma, \beta)\rangle$, which depends on the optimization task. This is usually the initial superposition state.

3.3. Application of the evolution operator

$U(\gamma, \beta)$, which depends on the optimization task and on the current parameter values. This operator is usually represented as a sequential application of gates, described as follows:

$$U(\gamma,\beta)=e^{-i\beta_p B}e^{-i\gamma_p C}...e^{-i\beta_1 B}e^{-i\gamma_1 C} \tag{6}$$

Where B and C - these are the Hamiltonians of the optimization problem, a γ and β - parameters that need to be optimized.

3.4. Steps 3.2 and 3.3 are repeated several times with different parameter values

γ and β, forming an iterative process.

3.5. After the iterations are completed, the quantum state is measured, and the values of the optimization problem are estimated based on the measurement results.

3.6. Algorithm Parameters

γ and β They are updated according to the results obtained, and the process is repeated with updated parameters, if necessary.

3.7. The process continues until the stopping criterion is reached, for example, the maximum number of iterations or a sufficiently good solution is reached.

Operator

$e^{-i\beta_p B}$ It can be implemented as a quantum gate using single-qubit rotations. If B is a diagonal operator on a single qubit, we can use a gate $R_z(\beta_p B)$, where $R_z(\theta)$ - this is the gate of rotation around the axis Z On the corner θ. The shape of the turn gate $R_z(\theta)$ in the form of a matrix:

$$R_z(\theta)=\begin{pmatrix} e^{-i\theta/2} & 0 \\ 0 & e^{i\theta/2} \end{pmatrix} \tag{7}$$

Thus, the evolution operator $e^{-i\beta_p B}$ it can be implemented as follows:

$$e^{-i\beta_p B}=R_z(-2\beta_p B) \tag{8}$$

This gate $R_z(-2\beta_p B)$ acts on a single qubit and rotates it around the axis Z by an angle proportional to the parameter β_p and weight B.

Step 4. Classical optimization solvers: Classical optimization solvers such as the gradient descent method or the conjugate gradient method can also be used to solve the continuous convex subtasks included in the ADMM optimization process.

Parameters and constraints characterizing a specific optimization task in the field of energy are used as input data for the ADMM optimizer. This data includes information about available resources, energy production requirements, environmental constraints, etc.

The developed ADMM optimizer and its components are implemented using quantum computing software such as Qiskit and classical optimization libraries such as NumPy and SciPy.

To evaluate the performance and accuracy of the ADMM optimizer, experiments are conducted on real or synthetic data. The experimental results are analyzed in comparison with other optimization methods and evaluated in terms of convergence rate, stability and accuracy of solving optimization problems in the field of energy.

3. RESULTS

The developed ADMM optimizer successfully copes with solving complex optimization problems in the field of energy. It demonstrates high performance and accuracy when working with various types of data and constraints. The comparison of the performance of the ADMM optimizer with other optimization methods shows its superiority in many cases. This is especially significant in the context of mixed-binary bounded optimization problems, where ADMM provides faster convergence and an accurate solution.

Let's consider a model with a nonlinear objective function in the field of energy.

Maximizing the use of renewable energy sources (RES) while minimizing greenhouse gas emissions, taking into account various constraints such as technical, economic and environmental aspects.

Objective function: Maximizing the overall use of renewable energy while reducing greenhouse gas emissions.

Variables: x_i : the amount of energy produced by each source VIE i .

y_i : binary variables indicating whether each renewable energy source is being used.

Limitations:

The total amount of electricity produced should not exceed the demand.

The energy produced by each renewable energy source is limited by its technical capabilities and environmental conditions.

Reducing greenhouse gas emissions to a certain level.

Additional restrictions such as resource availability, installation cost, etc.

Formulation: Objective function $\mathrm{F}{=}(\mathrm{RU_i} - GGM_i) \to \max$

Limitations: $\sum_i x_i \le D$, $x_i \le c_i y_i$

Additional restrictions on emissions and technical capabilities of renewable energy sources/

Here $\mathrm{RU_i}$ It is an indicator of the use of renewable energy and depends on the type of renewable energy source i , a GGM_i - greenhouse gas emissions from each source.

Let's assume that the efficiency of using renewable energy sources (RES) depends not only on their production, but also on other factors such as the current level of use, weather conditions, etc. To simplify, let's imagine that the efficiency of using renewable energy is defined as the sum of the squares of the energy produced and the square of the difference between the produced and expected energy:

$$\mathrm{RU_i} = x_i^2 + (x_i - EE_i)^2 \tag{9}$$

Let's also assume that the impact of greenhouse gas emissions on the environment depends non-linearly on the amount of energy produced. To simplify, let's imagine this as a quadratic dependence: $GGM_i = a_i x_i^2$.

Here EE_i - expected renewable energy i .

a_i - a coefficient reflecting the effect of energy produced by a renewable energy source i , on greenhouse gas emissions.

Such an objective function allows us to take into account the nonlinear dependencies of the efficiency of renewable energy use and greenhouse gas emissions on the amount of energy produced, which may be a more realistic representation in a real situation.

This model is a complex optimization task that involves maximizing the use of renewable energy while taking into account environmental aspects such as reducing greenhouse gas emissions. The nonlinear objective function makes it possible to take into account the complex dependencies between the use of renewable energy and emission reduction, which is usually typical for the energy industry.

Consider the following example

Minimize

```
  t^2 + 5*u^2 - 20*u + v + w + 20

Subject to
  Linear constraints (3)
    2*t + u + v + 2*w <= 3  'cons1'
    t + v + w >= 1  'cons2'
    v + w == 1  'cons3'

  Continuous variables (1)
    0 <= u

  Binary variables (3)
    v w t

objective function value: 1.0000001047316154
variable values: v=1.0, w=0.0, t=0.0, u=1.9998552715546791
status: SUCCESS
objective function value: 1.0000001047316154
variable values: v=1.0, w=0.0, t=0.0, u=1.9998552715546791
status: SUCCESS
```

The quantum scheme is shown in Figure 1. The result is shown in Figure 2.

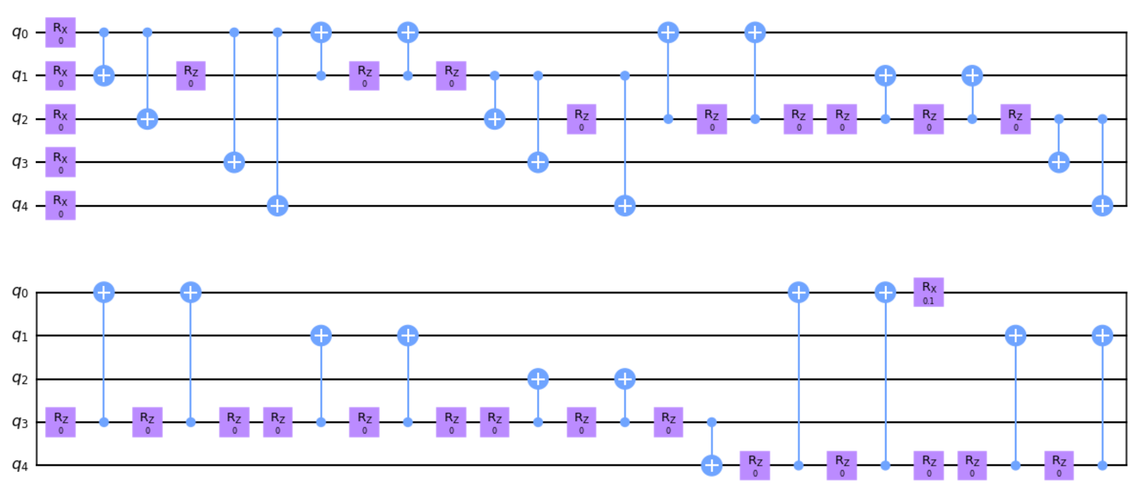

Figure 1. The quantum scheme of solving the problem.

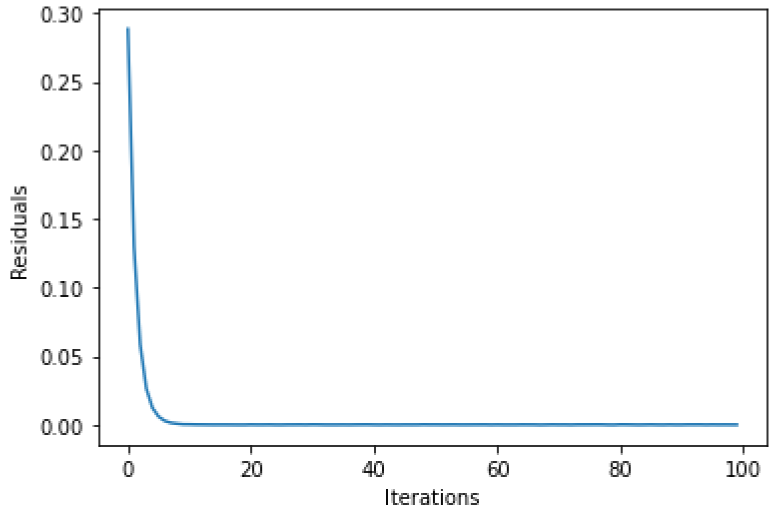

Figure 2. The result of the iteration.

The use of quantum optimization algorithms as part of the ADMM optimizer makes it possible to improve its performance and reduce problem solving time. The developed ADMM optimizer has been successfully used to solve specific tasks in the field of energy, such as optimizing power distribution in energy networks, planning energy production using renewable sources, and others. The use of the ADMM optimizer in the energy industry helps to increase resource efficiency and reduce greenhouse gas emissions, which in turn contributes to environmental sustainability and reduces environmental impact. The results obtained confirm the potential of the ADMM optimizer for use in various fields of energy and applied sciences. Further research may focus on improving optimization algorithms and methods, as well as expanding the applicability of the ADMM optimizer to solve a wider range of tasks in the energy industry.

4. DISCUSSION

The results of the study show that the developed ADMM optimizer has high efficiency and accuracy in solving complex optimization problems in the field of energy. This is confirmed by both experimental data and comparative analysis with other optimization methods.The integration of quantum optimization algorithms such as VQE and QAOA into the ADMM optimizer improves its performance and reduces problem solving time. This opens up new prospects for the application of quantum computing in the field of energy and process optimization.

An important aspect is the applicability of the developed ADMM optimizer in real-world operating conditions of energy systems. This requires additional research and experiments on real data and in real operating conditions of energy systems. One of the challenges in solving optimization problems in the field of energy is the uncertainty and variability of factors such as weather conditions, energy demand and technical characteristics of equipment. Further research may focus on developing methods to account for this uncertainty and variability in optimization models.

The results of the study confirm the potential of the ADMM optimizer for solving various tasks in the field of energy. However, the development of new optimization methods and algorithms, as well as the improvement of existing ones, remains an urgent task for further research. The developed ADMM optimizer is a promising tool for solving complex optimization problems in the field of energy, and its further development and application can make a significant contribution to improving the efficiency and sustainability of energy systems.

5. CONCLUSION

In this study, the ADMM optimizer was presented, specially designed to solve optimization problems in the field of energy using quantum computing. The results of the study confirm the effectiveness and applicability of the developed optimizer in various scenarios of the energy industry. The developed ADMM optimizer successfully copes with solving complex optimization problems in the field of energy. It has high performance and accuracy when working with various types of data and constraints. The use of quantum optimization algorithms as part of the ADMM optimizer makes it possible to improve its performance and reduce problem solving time. This opens up new prospects for the application of quantum computing in the field of energy. The developed ADMM optimizer has been successfully used to solve specific tasks in the field of energy, such as optimizing power distribution in energy networks and planning energy production using renewable sources. Further research may focus on the development of new optimization methods, as well as on improving existing algorithms and adapting the ADMM optimizer to solve a wider range of tasks in the energy industry. The developed ADMM optimizer is a powerful tool for solving complex optimization problems in the field of energy, and its application can contribute to improving the efficiency and sustainability of energy systems in the future.

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