VARIATIONAL QUANTUM ALGORITHMS FOR EUCLIDEAN DISCREPANCY AND COVARIATE-BALANCING

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Abstract. Algorithmic discrepancy theory seeks efficient algorithms to find those two-colorings of a set that minimize a given measure of coloring imbalance in the set, its discrepancy. The Euclidean discrepancy problem and the problem of balancing covariates in randomized trials have efficient randomized algorithms based on the Gram-Schmidt walk (GSW). We frame these problems as quantum Ising models, for which variational quantum algorithms (VQA) are particularly useful. Simulating an example of covariate-balancing on an IBM quantum simulator, we find that the variational quantum eigensolver (VQE) and the quantum approximate optimization algorithm (QAOA) yield results comparable to the GSW algorithm.

1. Introduction

A broad description of discrepancy theory given in [1] is that it is the theory of the irregularities of distributions. Precise formulations of discrepancy depend on the spaces and sets being studied (for a comprehensive treatment, see [1, 2]). To motivate this discussion, consider a finite discrete set $P$. We are given a collection $\mathcal{S}$ of subsets of $P$, constituting a set-system $(P, \mathcal{S})$. Let $\omega$ be a two-coloring of $P$ given by a map from $P$ to $\{+1, -1\}$,

$$\omega : P \rightarrow \{+1, -1\}.$$ 

For a set $S \in \mathcal{S}$ and a coloring $\omega$, let the absolute difference in the number of elements in $S$ colored $+1$ and $-1$ be,

$$d_S(\omega) = \left| \sum_{p \in P \cap S} \omega(p) \right|.$$ 

Define the coloring-discrepancy of the coloring $\omega$ as the maximum of this difference, over all $S \in \mathcal{S}$,

$$d_S(\omega) = \max_{S \in \mathcal{S}} d_S(\omega).$$
Then the discrepancy of the set system \((P, S)\) is defined as
\[
\text{disc}(S) = \min_{\omega} d_S(\omega).
\]

Beck and Fiala [3] established a highly regarded bound on discrepancy in discrete spaces. Spencer [4] subsequently obtained the famed “six standard deviations” result. The definition of discrepancy is expanded from above in spaces with more structure. Bárány and Grinberg [5] derived results on vector spaces with discrepancy quantification via seminorms. Banaszczyk [7] proved strong bounds for Euclidean discrepancy and in [6] generalized the results of Beck and Fiala [3] to vector balancing in convex bodies.

Recent accomplishments in algorithmic discrepancy theory realizing efficient algorithms for colorings which had previously been proven only to exist, began with Bansal’s [8] algorithm for Spencer’s result [4]. It allows efficient sampling of colorings with strongly bounded discrepancy, previously considered computationally hard. Bansal et al [9] have also developed an efficient randomized algorithm, the Gram-Schmidt Walk (GSW) algorithm, that samples colorings in Banaszczyk’s Theorem [6] and several others. This has been refined to tighter bounds, and extended in both theoretical and algorithmic directions, in the work of Harshaw et al [10] on covariate balancing.

In the current era of Noisy Intermediate-Scale Quantum (NISQ) devices [11], Variational Quantum Algorithms (VQA), also called hybrid quantum-classical algorithms, find much use. The main VQA are the Variational Quantum Eigensolvers (VQE) [12, 13] and the Quantum Approximate Optimization Algorithm (QAOA) [14], both of which have been shown to be very effective in approximating solutions to certain optimization problems [15], and approximating the ground state energies (minimum eigenvalues) of Hamiltonians [16–19].

In the present paper, we focus on a restricted version of discrepancy in [5, 6, 10], on a finite dimensional real vector space with Euclidean norm. This is naturally suited to quantum algorithms which assume a complex vector space with inner product norm. It also lends itself to the connection with the Ising model [20], and thus to VQA.

The rest of this paper is organized as follows. Section 2 introduces Euclidean discrepancy and the theorem of Banaszczyk [7] that sets bounds on it. Section 3 is a very brief description of the variational quantum algorithms (VQA) and Hamiltonians for Ising models. Section 4 discusses the Quadratic Unconstrained Signed Optimization (QUSO). Section 5 sets up the Ising model for the Euclidean discrepancy and covariate-balancing from [10], explaining the context of randomized trials. With this formulation, these problems are accessible by the VQA. Section 6 then tests the widely used variational quantum algorithms, Variational Quantum Eigensolvers (VQE) and the Quantum Approximate Optimization Algorithm (QAOA), on a quantum simulator to sample assignments for a test case. The experiments confirm the ability of these quantum algorithms, on that example, to sample assignments that perform well relative to the GSW algorithm. Section 7 is the conclusion.

2. Euclidean discrepancy

In this setting, we have \(\mathbb{R}^n\) as the ambient space, and a set of \(m\) vectors \(X = \{x_1, \ldots, x_m \in \mathbb{R}^n\}\). Let the coloring-discrepancy be the map from the space of colorings \(\{\omega_1, \ldots, \omega_m = \pm 1\}\) to \(\mathbb{R}\),

\[
d_X(\omega) = \left\| \sum_{i=1}^{m} \omega_i x_i \right\|,
\]
where $\|\cdot\|$ is the Euclidean norm. The Euclidean discrepancy of the set of vectors $X = \{x_1, \ldots, x_m \in \mathbb{R}^n\}$ is

$$\text{disc}(X) = \min_{\{\omega\}} \{d_X(\omega)\}. \quad (2)$$

A coloring $\omega^*$ is called an optimal coloring if

$$d_X(\omega^*) = \text{disc}(X). \quad (3)$$

Let us recall a theorem of Banaszczyk [7].

**Theorem 2.1** (Banaszczyk [7]). Let $D$ be an $n$-dimensional ellipsoid in $\mathbb{R}^n$ with center at 0 and principal semi-axes $\lambda_1, \ldots, \lambda_n$. Choose any $x_1, \ldots, x_m \in D$ ($m$ is arbitrary, independent of $n$). Then:

(a) there exist signs $\omega_1, \ldots, \omega_m = \pm 1$, such that

$$\left\| \sum_{i=1}^{m} \omega_i x_i \right\| \leq \left( \sum_{j=1}^{n} \lambda_j^2 \right)^{\frac{1}{2}},$$

(b) to each $k = 1, \ldots, m$ there corresponds a subset $I$ of $\{1, \ldots, m\}$ consisting of exactly $k$ elements, such that

$$\left\| \sum_{i \in I} x_i - \frac{k}{m} \sum_{i=1}^{m} x_i \right\| \leq \left( \sum_{j=1}^{n} \lambda_j^2 \right)^{\frac{1}{2}}.$$

In the above theorem, when the ellipsoid is a unit ball in $\mathbb{R}^n$, the right side of the inequalities become $\sqrt{n}$. \(^1\)

Let $X$ be the $n \times m$ matrix formed by using the vectors $\{x_i\}$ as column vectors,

$$X = \begin{bmatrix} x_1 & \cdots & x_m \end{bmatrix}. \quad (4)$$

Let us also write $\omega_1, \ldots, \omega_m$ as a column vector $\omega$,

$$\omega = \begin{bmatrix} \omega_1 \\ \vdots \\ \omega_m \end{bmatrix}. $$

Then we can write the square of coloring-discrepancy in eq. (1) as,

$$d_X(\omega)^2 = \omega^\top X^\top X \omega. \quad (5)$$

By the above theorem part [a] there exists a vector $\omega \in \{-1, 1\}^m$ such that $\|X \omega\| \leq \sqrt{n}$. This implies

$$d_X(\omega)^2 = \omega^\top X^\top X \omega \leq n.$$

\(^1\)Banaszczyk [7] attributes this special case to the earlier works of Sevastyanov [21] and Bárány (unpublished).
3. Variational quantum algorithms and the Ising model

We give a short introduction to the Ising model and the VQA, the first being a core object in this paper, and the second being the paradigmatic tool that realizes the optimization we need.

Let $H$ be a Hilbert space of $m$ qubits,

$$H = \mathbb{C}^{2^{\otimes m}}.$$ \hfill (6)

In the usual notation, let the standard basis vectors of $\mathbb{C}^2$ be

$$|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad |1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

Then a natural basis of $H$ is the product-basis,

$$\mathcal{B} = \left\{ \bigotimes_{i=1}^{m} |b_i\rangle : b_i = 0, 1 \right\}.$$

A Hamiltonian $H$ is a self-adjoint operator on $H$, which, for the current discussion, which is expressible as sum of chains of Pauli spin matrices on $H$. By way of explanation, Pauli spin matrices are

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}.$$ \hfill (7)

Let

$$\sigma_0 = \mathbb{I}_2 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

be the $2 \times 2$ identity matrix. For a multi-index $I = (i_1, \ldots, i_m)$, $i_j \in \{0, x, y, z\}$, let

$$\sigma_I = \sigma_{i_1} \otimes \cdots \otimes \sigma_{i_m}.$$ \hfill (7)

Any Hamiltonian $H$ may be written as

$$H = \sum_{I \in \mathcal{I}_H} \alpha_I \sigma_I,$$

where $\mathcal{I}_H \subset \{0, x, y, z\}^{\times m}$, and $\alpha_I$ are some real values. In an Ising model Hamiltonian [20], the multi-index set $\mathcal{I}$ consists of those $I = (i_1, \ldots, i_m)$ with either 1 or 2 of the subindices $i_k = z$, and the remaining 0, i.e., it has 1 or 2 of the $\sigma_{i_k} = \sigma_z$ in eq. (7) and the rest are $\mathbb{I}_2$.

In a more familiar notation, an Ising model Hamiltonian can be written as

$$H = \sum_{i, j} \alpha_{ij} \sigma_i^z \sigma_j^z + \sum_k \beta_k \sigma_k^z,$$

where $\alpha_{ij}$ and $\beta_k$ are real, and

$$\sigma_i^z = \mathbb{I}_2 \otimes \cdots \otimes \mathbb{I}_2 \otimes \sigma_z \otimes \mathbb{I}_2 \otimes \cdots \otimes \mathbb{I}_2.$$ \hfill (8)

Let $\theta = (\theta_1, \ldots, \theta_r)$ be a set of real parameters, and let $|\psi(\theta)\rangle$ be a parametrized state (unit vector) in $H$. Then a variational quantum algorithm tries to minimize the mean value of $H$: $\langle \psi(\theta) | H | \psi(\theta) \rangle$, over the set of values of $\theta$. It is clear that

$$\langle \psi(\theta) | H | \psi(\theta) \rangle \geq \lambda_0,$$

where $\lambda_0$ is the minimum eigenvalue of $H$. If equality is attained in the above for some set of parameters $\theta^*$, then $|\psi(\theta^*)\rangle$ is an eigenvector of $H$ with the eigenvalue $\lambda_0$. 

The quantum approximate optimization algorithm, QAOA [14], has been shown in [14] to approximately find the minimum (or the maximum as the case may be) of a class of combinatorial optimization problems. As QAOA are a specialized form of the more general VQE, that entails the same for the VQE. Ultimately, it is an attestation of their convergence to the minimum eigenvalues of Hamiltonians including the type we are concerned with. VQE convergence [13, 15] depends on the parametrized state $|\psi(\theta)\rangle$, called the variational ansatz, and the classical optimizer that adjusts the parameters $\theta$ during the search for the minimum eigenvalue (ground state) of the Hamiltonian. QAOA [14,17,18] gains by a state preparation circuit with an adjustable number ($p$) of layers of parametrized gates that are based on the Hamiltonian whose ground state is being sought. This structure makes it better adapted to the Hamiltonian and capable of converging to the ground state in the large $p$ limit [14, 17].

4. Quadratic Unconstrained Signed Optimization

Let us recall the definition of a quadratic unconstrained signed optimization (QUSO) problem. Let $Q$ be a positive symmetric $m \times m$ matrix.

**Definition 4.1 (Quadratic unconstrained signed optimization (QUSO) problem).** Let

$$h(\omega) = \omega^\top Q \omega,$$

where $\omega \in \{-1, 1\}^m$. (8)

The object of the problem is to find the minimum value $h_{\text{min}} = \min_{\omega \in \{-1, 1\}^m} h(\omega)$, and an element $\omega^* \in \{-1, 1\}^m$ minimizing $h$, i.e., $h(\omega^*) = h_{\text{min}}$.

Here, $h$ is called the **objective function**. The problem can be written as

$$\text{minimize } h(\omega) = 2 \sum_{i<j} Q_{ij} \omega_i \omega_j + \text{tr}(Q),$$

subject to $\omega_1, \ldots, \omega_m = \pm 1$, (9)

where $Q_{ij}$ is the $i,j$ entry of $Q$. This can be transformed to an Ising Hamiltonian as follows. Let us consider the complex Hilbert space as in eq. (6),

$$\mathcal{H} = \mathbb{C}^{2^\otimes m}.$$

We set aside the constant offset, $\text{tr}(Q)$, in (9), mapping the quadratic sum to an Ising Hamiltonian,

$$H = 2 \sum_{i<j} Q_{ij} \sigma_i^z \sigma_j^z.$$ (10)

Note that $|0\rangle, |1\rangle$ are the eigenvectors of $\sigma_z$ with the eigenvalues 1, −1, respectively. Define the binary variables $y_i = (\omega_i + 1)/2$. Then each basis vector of $\mathcal{H}$ of the form

$$|y\rangle = \bigotimes_{i=1}^m |y_i\rangle = \bigotimes_{i=1}^m \left| \omega_i + 1 \right| 2 \right\rangle$$ (11)

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2There is no assertion here about the rate of convergence or the approximation error decay with the number of steps of the algorithm, i.e., its complexity.
is an eigenvector of the Ising Hamiltonian $H$. We call such an eigenvector a \textit{product-basis eigenvector}. Further, if we denote $\lambda_y$ to be the eigenvalue for the eigenvector $|y\rangle$, then

$$\lambda_y = \omega^\top Q \omega - \text{tr}(Q) = h(\omega) - \text{tr}(Q), \quad (12)$$

where $h$ is the objective function of eq. (8). Let us state this as a theorem, \footnote{Note that the form $\omega^\top Q \omega$ is invariant under the reflection $\omega \mapsto -\omega$, therefore, the map in eq. (11) does not affect the signs in eq. (12).}

**Theorem 4.2.** Let $Q$ be an $m \times m$ positive symmetric matrix. Let $h$ be the objective function in eq. (8) and $H$ be the Ising Hamiltonian in (10), each constructed from $Q$. Then there is a bijection

$$\gamma: (\omega, h(\omega)) \leftrightarrow (y, \lambda_y),$$

where $y$ and $\lambda_y$ are as in eqs. (11) and (12), respectively.

The obvious corollary is

**Corollary 4.3.** Let $Q$ be an $m \times m$ positive symmetric matrix. A quadratic unconstrained signed optimization (QUSO) problem (Definition 4.1) with $h$ in eq. (8) as its objective function is equivalent to the problem of finding the minimum eigenvalue, and a corresponding product-basis eigenvector of the Hamiltonian $H$ in (10).

5. Ising models for Euclidean discrepancy and covariate-balancing

Let $x_1, \ldots, x_m \in \mathbb{R}^n$ be an arbitrary set of vectors and let $X$ be the matrix in eq. (4) using them as columns. Let $Q_X = X^\top X$. We can rewrite the (square of) coloring-discrepancy in eq. (5) as

$$h_X = d_X(\omega)^2 = \left\| \sum_{i=1}^m \omega_i x_i \right\|^2 = \omega^\top Q_X \omega.$$

Then the search for the Euclidean discrepancy given by eq. (2) and an optimal coloring satisfying eq. (3), is a QUSO problem with the objective function $h_X$. Let us convert $h_X$ to an Ising Hamiltonian,

$$H_X = 2 \sum_{i<j} Q_{X_{ij}} \sigma_i^z \sigma_j^z. \quad (13)$$

Covariate-balancing considers the problem of assigning subjects in a randomized trial to two groups so that there is a degree of \textit{robustness} against the worst-case error, specified by a parameter, that trades it with balancing the covariates among the groups. The algorithm in [10] for covariate balancing in randomized trials, makes use of the Gram-Schmidt walk algorithm of [9]. Let an $n \times m$ matrix $X$ be the $n$-dimensional covariate (row) vectors of $m$ subjects in an experimental study. Assume the vector $\omega \in \{-1, +1\}^m$ represents the assignment of the $m$ subjects enumerated by $i = 0, \ldots, m-1$ to one of two possible \textit{treatment} groups under the experiment, grouped by the sign $\omega_i = \pm 1$. For a random vector $v \in \mathbb{R}^k$, for any $k$, denote its covariance matrix by $\text{Cov}(v) = E(vv^\top)$, where $E$ denotes the expected value over the distribution from which $v$ is sampled. The algorithm in [10] has the flexibility to trade-off balance, embodied in $\text{Cov}(X\omega)$, with robustness, which would best be attained
by making \( \text{Cov}(\omega) = I_m \). The \((m+n) \times m\) augmented covariate matrix \( B \) in [10] trades off these through a parameter \( \phi \),

\[
B = \begin{bmatrix}
    \sqrt{\phi}I_m \\
    \xi^{-1}\sqrt{1 - \phi}X
\end{bmatrix},
\]

where \( I_m \) is an \( m \times m \) identity matrix. The parameter \( \phi \in [0,1] \) determines the degree to which the vector \( \omega \) approximates either the result of raw covariates given by \( X \) or that from the pairwise independent assignments coming from \( I_m \). The parameter \( \xi = \max_{i\in[m]} \|x_i\| \) ensures that the two matrices have equal influence in contributing to \( \omega \). For the rest of this section, fix the parameter \( \phi \). We will call the colorings \( \omega \) that minimize \( \|B\omega\| \) as optimal covariate-balancing colorings for the matrix \( B \).

Write \( B \) as column vectors \( b_1, \ldots, b_m \in \mathbb{R}^{m+n} \),

\[
B = \begin{bmatrix}
    \vdots & \cdots & \vdots \\
    b_1 & \cdots & b_m \\
    \vdots & \cdots & \vdots
\end{bmatrix},
\]

where

\[
b_i = \begin{bmatrix}
    \sqrt{\phi}e_i \\
    \xi^{-1}\sqrt{1 - \phi}x_i
\end{bmatrix},
\]

and \( e_i \) is the \( i \)th standard coordinate vector in \( \mathbb{R}^m \). Define the assignment-imbalance,

\[
i_X : \{-1, 1\}^m \rightarrow \mathbb{R}
\]

\[
i_X(\omega) = \left\| \sum_{i=1}^m \omega_i b_i \right\|
\]

Taking the minimum over \( \omega \) of the assignment-imbalance, we can define the augmented-imbalance\(^5\) as

\[
\text{imb}(X) = \min_{\{\omega\}} i_X(\omega).
\]

An optimal assignment \( \omega^* \) as one that achieves the augmented-imbalance,

\[
i_X(\omega^*) = \text{imb}(X).
\]

And as in the case of the Euclidean discrepancy, define the matrix

\[
Q_B = B^\top B.
\]

We can rewrite the square of the assignment-imbalance as

\[
h_B(\omega) = i_X(\omega)^2 = \omega^\top Q_B \omega.
\]

The problem of finding an optimal assignment and the augmented-imbalance is then a QUSO problem with the objective function \( h_B \). Converting \( h_B \) to an Ising Hamiltonian, we have

\[
H_B = 2 \sum_{i<j} Q_{Bij} \sigma_i^z \sigma_j^z.
\]

Then, by Corollary 4.3, we have

**Theorem 5.1.** Given a set of vectors \( x_1, \ldots, x_m \in \mathbb{R}^n \),

\(^5\)The authors are unaware of the proper terminology here.
(a) finding their Euclidean discrepancy given by eq. (2) and an optimal coloring given by eq. (3) is equivalent to finding the minimum eigenvalue, and a corresponding product-basis eigenvector of the Ising Hamiltonian $H_X$ in eq. (13).

(b) finding their augmented-imbalance given by eq. (14), and an optimal assignment given by eq. (15) is equivalent to finding the minimum eigenvalue, and a corresponding product-basis eigenvector of the Ising Hamiltonian $H_B$ in eq. (16).

The constructions and results in [10] provide extensive analysis, bounds and criteria quantifying performance, implications and complexity of the algorithm. From a much simplified and coarse perspective, the algorithm samples from $\omega$ such that the largest eigenvalue of $\text{Cov}(B\omega)$ is close to the minimum that it can be over all $\omega \in \{-1,1\}^m$. Let us see how this behaves in the variational quantum algorithms case. A variational quantum optimizer samples the vector $\omega$ (equivalently $|y\rangle$ in eq. (11)) from the values that make $E(\|B\omega\|^2)$ close to the minimum. A useful observation is that $\|B\omega\|^2 = \text{tr}(B\omega\omega^T B^T)$, which implies that $E(\|B\omega\|^2) = \text{tr} \text{Cov}(B\omega) = \sum_{k=1}^{m} \lambda_k$, where $\lambda_k$ are the eigenvalues of $\text{Cov}(B\omega)$. This means that the largest eigenvalue of $\text{Cov}(B\omega)$ will be close to the minimum it can be over all $\omega \in \{-1,1\}^m$.

When $\phi = 0$, $Q_B = X^T X$, which is the same as in the previous section. When $\phi = 1$, $Q_B = I_m$. All of the eigenvalues of $Q_B$ are 1. Then a VQE capable of sampling from the entire space, would sample $\omega$ uniformly from all its possible values, resulting in $\text{Cov}(B\omega) = \text{Cov}(\omega) = I_m$.

Sometimes it might be desirable to have the same number of +1’s as −1’s in the optimal assignment, i.e., that the number of subjects are split equally into the treatment groups. This is called the group-balanced randomization design in [10]. For that, the particle-number preserving ansatz from [22], with $m/2$ particles, may be used in the variational algorithm. We leave the details of the proper ansatz choice from the cited work to the interested reader. In the next section, we test the VQA on an IBM quantum device simulator to see if they work as expected.

6. Running variational quantum algorithms on quantum simulators

Here we demonstrate, using a simple example, the variational quantum algorithm for covariate balancing. We run the algorithm on IBM quantum (qasm) simulator [23] with the code written in the IBM Qiskit [24] framework, and compare the result with the algorithm in [10]. The code for the algorithm in [10] is available as a repository [25]. Publicly accessible IBM quantum simulators have the VQE and QAOA routines available, and we use them, indicating the parameter settings, but without describing what they mean. The reader is referred to the online resources within IBM Qiskit [24], or to the several papers we have cited on the topics [12–14, 17–19].

The experiment we conduct is limited by the resources available. The dimensions of the multi-qubit Hilbert space grows exponentially with $m$, the number of covariate vectors, i.e., the number of subjects in the trial. The purpose of this experiment is to demonstrate the variational quantum algorithms approach. We generate $m = 12$ covariate vectors, $\{x_i \in \mathbb{R}^2\}$, drawn evenly from 2 Gaussian distributions with means $[-3,3]$ and $[3,3]$, and variances 1 in each coordinate direction. These are shown in figure 1 and given as the matrix $X$ in 6The code is available upon request.
Appendix A, eq. (17). The parameter balance-robustness parameter $\phi = 0.5$ for all the assignments that follow, except, naturally, for the uniformly random assignment.

Let us assign these vectors to two groups, i.e., sample the assignment vector $\omega \in \{\pm 1\}^m$ using some randomized method.

**Uniformly random.** The entries $\omega_i = \pm 1$ are chosen independently and uniformly randomly. The sampled $\omega$ is in eq. (18). Figure 2 shows the assignment of each vector $x_i$ to the corresponding treatment group $\omega_i$. We observe that the each group is “clumped” in one of the two distributions.

**GSW.** Next we sample the assignment based on the GSW algorithm described in [10] implemented in the code repository [25]. We obtain a sample $\omega$ given in eq. (19), after a few runs that attains the best observed assignment-imbalance value $i_X(\omega) = 2.4720$. The assignment to treatment groups is shown in figure 3.
VQE. We test the VQE algorithm of IBM Qiskit [24] with the setup of Section 5. From VQE we get a sample $\omega$ given in eq. (20), with the assignment-imbalance value $i_X(\omega) = 2.4497$. Figure 4 shows the sampled assignment.

QAOA. We test the QAOA algorithm of IBM Qiskit [24], for the same setup as for VQE. This yields a sample $\omega$ given in eq. (21), with the assignment-imbalance value $i_X(\omega) = 2.4516$. The assignment is displayed in figure 5.

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7The simulation runs 65536 shots on the qasm-simulator backend. It uses the two-local variational ansatz, with rotation-blocks: \{“rz”, “ry”\}, entanglement-blocks: “cx”, reps: 3, entanglement: “circular”. The rest of the parameters are the default ones. The optimizer used is the Constrained Optimization by Linear Approximation optimizer (COBYLA).

8This simulation runs 65536 shots on the qasm-simulator backend. It uses $p = 8$, with a uniform superposition initial state. The optimizer used is the Constrained Optimization by Linear Approximation optimizer (COBYLA).
Optimal by exhaustive search. As a comparison, we also find, through exhaustive search, the imbalance $\text{imb}(X)$ (minimum assignment-imbalance value), and an optimal assignment. The optimal $\omega$ we find is given in eq. (22), and the imbalance is $\text{imb}(X) = i_X(\omega^*) = 2.4496$. Figure 6 shows the optimal assignment.

7. Conclusion

Posing the classical problems of Euclidean discrepancy and covariate balancing as QUSO problems allows us to convert them to Ising models. This turns the search for optimal colorings and assignments of subjects in randomized trials to the search for the lowest eigenvalues of Ising Hamiltonians. These are precisely the problems for which the VQA, in particular the VQE and the QAOA, have been developed and furnish powerful approaches to optimization in the NISQ regime of quantum computing. The experiment in the previous section demonstrates the efficacy of using the VQA in this search, whose performances compare favorably, though for a modest example, to the GSW algorithm. We realize the need for extensive tests, especially on actual quantum devices, to draw meaningful comparisons. Within covariate-balancing, different parameters values could be tested, and so could constrained
optimizations such as the group-balanced randomization design, for which we cited a possible VQE ansatz from the extant literature. Future work may seek to expand the VQA to other aspects of algorithmic discrepancy theory. Another interesting, and indeed potentially unexplored, direction is the investigation of efficient quantum algorithms for discrepancy theory, with the recent discoveries in classical algorithms for it serving as a motivation and as possible guides.

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Appendix A. Numerical simulation data

Matrix of covariates (transpose):

\[
X^\top = \begin{bmatrix}
3.8673 & 2.0983 \\
2.5055 & 2.0971 \\
3.8644 & 5.2119 \\
3.5328 & 2.7283 \\
3.5023 & 2.4830 \\
2.4395 & 2.9807 \\
-2.8719 & 4.8528 \\
-3.8278 & 3.1101 \\
-3.2512 & 3.3697 \\
-2.9279 & 1.4966 \\
-1.4358 & 1.6033 \\
-1.8945 & 1.8933 \\
\end{bmatrix}\]  \quad (17)

Uniformly randomly sampled \( \omega \):

\[
\omega = [1, 1, 1, 1, -1, 1, -1, -1, 1, -1, 1, -1]. \]  \quad (18)

GSW sampled \( \omega \):

\[
\omega = [1, 1, -1, 1, -1, 1, 1, -1, 1, -1, 1, -1]. \]  \quad (19)

VQE sampled \( \omega \):

\[
\omega = [-1, -1, -1, 1, 1, -1, 1, 1, -1, 1, 1, -1]. \]  \quad (20)

QAOA sampled \( \omega \):

\[
\omega = [-1, -1, -1, 1, 1, -1, 1, -1, 1, 1, -1, 1]. \]  \quad (21)

Optimal \( \omega^* \) by exhaustive search:

\[
\omega^* = [1, -1, -1, 1, 1, -1, 1, 1, -1, 1, 1, -1]. \]  \quad (22)