Linear regression by quantum amplitude estimation and its extension to convex optimization

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Linear regression is a basic and widely used methodology in data analysis. It is known that some quantum algorithms efficiently perform least-squares linear regression of an exponentially large dataset. However, if we obtain values of the regression coefficients as classical data, the complexity of the existing quantum algorithms can be larger than the classical method. This is because it depends strongly on the tolerance error ϵ : the best one among the existing proposals is $O(\epsilon^{-2})$. In this paper, we propose a quantum algorithm for linear regression, which has a complexity of $O(\epsilon^{-1})$ and keeps a logarithmic dependence on the number of data points N_D . In this method, we overcome bottleneck parts in the calculation, which take the form of the sum over data points and therefore have a complexity proportional to N_D , using quantum amplitude estimation, and other parts classically. Additionally, we generalize our method to some class of convex optimization problems.

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I. INTRODUCTION

Following the rapid advance of quantum computing technology, many quantum algorithms have been proposed, and their applications to the wide range of practical problems have been studied in recent research. One prominent example is linear regression. Linear regression, which is based on the least-squares method in many cases, is a basic and ubiquitous methodology for many fields in natural and social sciences. There are some quantum algorithms for linear regression [1–6] with complexity depending on the number of data points N_D as $O(\text{polylog}(N_D))$.¹ This denotes the exponential speedup compared with the naive classical method explained in Sec. II B, whose complexity is proportional to N_D .

However, despite this, the existing quantum methods are not necessarily more beneficial than classical ones when we want to obtain the values of the optimized regression coefficients as classical data, and N_D is *midsized*, say, $O(10^3\text{--}10^5)$. Roughly speaking, in the existing methods such as the first proposed one [1], which is based on the Harrow-Hassidim-Lloyd (HHL) algorithm [10] for solving systems of linear equations, the authors create quantum states in which the values of the coefficients are encoded and read out in classical form. Therefore, it is inevitable that the estimated coefficients are accompanied by errors, and high-accuracy estimation leads to large complexity. As far as we know, the existing method with the best complexity with respect to the tolerance error ϵ is that in [3]: the complexity of estimating coefficients with additive error at most ϵ is

$$O\left(\frac{d^{5/2}\kappa^3}{\epsilon^2}\text{polylog}\left(\frac{d\kappa}{\epsilon}\right)\right), \quad (1)$$

where d is the number of the coefficients (or the explanatory variables) and κ is the condition number of the design matrix (defined in Sec. II B). On the other hand, a naive classical method has complexity, $O(d^2N_D)$. Therefore, assuming the prefactors in these expressions of complexities are comparable, under an ordinary situation $\epsilon \sim 10^{-3}$, $d \sim 10$, $\kappa \sim 1$, the minimum N_D for which the quantum method is advantageous over the classical one is $N_D \sim 10^6$. Although in some problems N_D is of such an order or much larger, cases in which $N_D \sim 10^3$ or 10^4 are also ubiquitous, and in such cases the existing quantum methods are inferior to the classical ones.

The midsized regression problems are often time-consuming and need to be sped up, although we might naively think that such problems can be solved by classical computers in a short time. For example, if such regressions are repeated in the whole of the calculation flow, the total computational time can be long. One such case is the *least-square Monte Carlo (LSM)* [11]. LSM is a methodology used in pricing financial derivatives² with an early exercise option, that is, the contract term stating that either of two parties in the contract can terminate it before final maturity.³ In Monte Carlo pricing, we generate many [say, $O(10^4\text{--}10^5)$] paths of the random time evolution of underlying assets, and we estimate the price as the expected cash flow. In the case of early exercisable products, we have to determine the optimal exercise time for each path. In LSM, we approximate the continuation value of the derivative at each exercise date by linear regression using certain functions of underlying asset prices as explanatory variables, whose number is typically $d \sim 10$. Since regression

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¹There are also quantum-inspired classical methods [7–9].

²Financial derivatives, or simply derivatives, are financial contracts in which two parties exchange cash flows whose amounts are determined by the price of some assets. For textbooks on derivatives and their pricing, we refer to [12,13].

³For the details of LSM, see [11].

is done many times in pricing one contract, and banks have numerous contracts, they have huge complexity in total and are meaningful targets of quantum speedup, even though each of them is midsized.

Based on the above motivation, in this paper we present a quantum algorithm for linear regression, focusing on reducing the order of the inverse of ϵ in the expression of the complexity. In our method, unlike existing methods, we do not perform all of the calculations on a quantum computer. Instead, we use a quantum computer *only to perform a bottleneck part in the naive classical method*. That is, we perform some intermediate calculation, which is the sum over N_D terms and therefore has complexity proportional to N_D naively, by quantum algorithm. Then, we classically solve the d -dimensional system of linear equations, whose coefficients and constant terms are outputs of the preceding quantum computation, and we obtain the regression coefficients. A classical computer can perform this step in negligible time for $d \sim 10$, without inducing any error. Also note that we naturally obtain the regression coefficients as classical data.

To speed up the bottleneck sums, we use *quantum amplitude estimation (QAE)* [14–20], which is also used to speed up Monte Carlo integration [15, 21]. Then, as discussed in detail in Sec. III, we can perform the sums with complexity,

$$O\left(\max\left\{\frac{d^{3/2}\kappa^4}{\epsilon}, d\kappa^2\right\} \times d^2 \ln(d)\right),$$

and the total complexity of the whole of our method is almost equal to this. Compared with the naive classical method, whose complexity is $O(d^2 N_D)$, our method accomplishes speedup with respect to N_D . In addition, compared with the existing quantum methods, our method improves the dependency of the complexity on ϵ from ϵ^{-2} in (1) to ϵ^{-1} . Unfortunately, in our method, the dependencies on d and κ are worse than those of (1) and the naive classical method. Therefore, our method is more suitable to the situation such that

$$d, \kappa \ll \frac{1}{\epsilon} \ll N_D, \quad (2)$$

which includes typical midsized problems such as LSM.

In addition to linear regression, we generalize our method to some class of convex optimization. As we see in Sec. IV, linear regression can be considered as an optimization problem of the sum of quadratic functions solved by Newton's method. Inspired by this, we consider a convex optimization problem where an objective function is written as sums of many terms similarly to linear regression, and we present a quantum algorithm of Newton's method, in which calculation of the gradient and the Hessian is sped up by QAE. We also estimate complexity to obtain a solution with a desired error level under some mathematical assumptions which are usually made in the convergence analysis of Newton's method.

The remaining parts of this paper are organized as follows. Section II is a preliminary section. In Sec. II A, we present some notations and definitions of quantities necessary for the later discussion. In Sec. II B, we briefly review linear regression and its classical method. In Sec. III, we explain our method in detail. In Sec. IV, we discuss the extension of

our method to some convex optimization problems. Section V summarizes the paper.

II. PRELIMINARY

A. Notations and definitions

In this subsection, we present some notations and definitions about linear algebra for later use. For details, refer to textbooks on linear algebra, e.g., Ref. [22].

For $\vec{v} = (v_1, \dots, v_n)^T \in \mathbb{R}^n$, we define the Euclidean norm $\|\vec{v}\|$ and the max norm $\|\vec{v}\|_\infty$ as follows:

$$\|\vec{v}\| := \sqrt{\sum_{i=1}^n |v_i|^2}, \quad \|\vec{v}\|_\infty := \max\{|v_1|, \dots, |v_n|\}. \quad (3)$$

We also define some types of norms for a matrix $A = (a_{ij})_{\substack{1 \leq i \leq m \\ 1 \leq j \leq n}} \in \mathbb{R}^{m \times n}$. The first one is the *spectral norm*, which is defined as

$$\|A\| := \max_{\substack{\vec{v} \in \mathbb{R}^n \\ \|\vec{v}\| \neq 0}} \frac{\|A\vec{v}\|}{\|\vec{v}\|}, \quad (4)$$

and equal to $\sigma_{\max}(A)$, the maximum singular value of A . Secondly, we define the *Frobenius norm* as

$$\|A\|_F := \left(\sum_{i=1}^m \sum_{j=1}^n |a_{ij}|^2 \right)^{1/2}, \quad (5)$$

which satisfies $\|A\| \leq \|A\|_F$.

Furthermore, we introduce the *condition number*, which measures the sensitivity of a linear operator to the errors in the input. For a full-rank matrix $A \in \mathbb{R}^{m \times n}$, the condition number is defined as

$$\kappa(A) := \frac{\sigma_{\max}}{\sigma_{\min}}, \quad (6)$$

that is, the ratio of the maximum singular value $\sigma_{\max}$ of A to the minimum one $\sigma_{\min}$. If A is invertible,

$$\kappa(A) = \|A\| \|A^{-1}\|. \quad (7)$$

B. Linear regression

We define here the problem of linear regression. Assume that we have N_D data points $\mathcal{D} := \{(\vec{x}_i, y_i)\}_{i=1, \dots, N_D}$, each of which consists of a vector of d explanatory variables⁴ $\vec{x}_i = (x_i^{(1)}, \dots, x_i^{(d)})^T \in \mathbb{R}^d$ and an objective variable $y_i \in \mathbb{R}$. Linear regression attempts to fit the linear combination of the explanatory variables to the objective variable, that is, finding $\vec{a}$ such that

$$\vec{y} \simeq X\vec{a}. \quad (8)$$

Here, $a_1, \dots, a_d \in \mathbb{R}$ are model parameters called *regression coefficients* and $\vec{a} := (a_1, \dots, a_d)^T \in \mathbb{R}^d$.

⁴If we want to consider the intercept, we include a dummy variable (say $x_i^{(1)}$) in each explanatory variable vector and set it to 1: $x_1^{(1)} = \dots = x_{N_D}^{(1)} = 1$.

$\vec{y} := (y_1, \dots, y_{N_D})^T$ and

$$X := \begin{pmatrix} x_1^{(1)} & \cdots & x_1^{(d)} \\ \vdots & \ddots & \vdots \\ x_{N_D}^{(1)} & \cdots & x_{N_D}^{(d)} \end{pmatrix} \quad (9)$$

is called the *design matrix*. In this paper, as in many cases, we determine $\vec{a}$ by the *least-squares method*, that is,

$$\vec{a} = \underset{\vec{a}'}{\operatorname{argmin}} \|\vec{y} - X\vec{a}'\|^2. \quad (10)$$

As is well known (again, see [22] for example), the solution of (10) is given by

$$\vec{a} = (X^T X)^{-1} X^T \vec{y}, \quad (11)$$

where we assume that X is full-rank, as stated again in Sec. III B as Assumption 2.

Here, let us introduce some symbols. We define $d \times d$ matrix W ,

$$W := \frac{1}{N_D} X^T X, \quad (12)$$

whose (i, j) -element is

$$w_{ij} = \frac{1}{N_D} \sum_{k=1}^{N_D} x_k^{(i)} x_k^{(j)}. \quad (13)$$

W is invertible since we assumed that X is full-rank. We also define the d -dimensional vector $\vec{z}$,

$$\vec{z} := \frac{1}{N_D} X^T \vec{y}, \quad (14)$$

whose i th element is

$$z_i = \frac{1}{N_D} \sum_{k=1}^{N_D} x_k^{(i)} y_k. \quad (15)$$

In (12) and (14), the prefactor $1/N_D$ is just for later convenience. Using these, (11) becomes

$$\vec{a} = W^{-1} \vec{z}. \quad (16)$$

Here we refer to the following classical computation as the *naive classical method*: calculate w_{ij} 's and z_i 's by simply repeating multiplications and additions N_D times, literally following the definitions (13) and (15), and then solve the d -dimensional system of linear equations (16) to find $\vec{a}$. Let us discuss the complexity of this method. Since we are considering the situation $d \ll N_D$, we focus only on the major contributions with respect to N_D . Calculating one w_{ij} or z_i takes a complexity of $O(N_D)$. Since the numbers of w_{ij} 's and z_i 's are $O(d^2)$ and $O(d)$, respectively, and their total is $O(d^2)$, the total complexity of calculating all of w_{ij} 's and z_i 's is $O(d^2 N_D)$. Then, solving (16) takes the negligible complexity, since it does not depend on N_D . For example, even if we use an elementary method such as row reduction, the complexity is $O(d^3)$. In summary, the complexity of the naive classical method is $O(d^2 N_D)$, which dominantly comes from calculation of w_{ij} 's and z_i 's.

III. LINEAR REGRESSION BY QUANTUM AMPLITUDE ESTIMATION

A. Quantum amplitude estimation

In this section, we present our method for linear regression. Before this, let us briefly review the outline of QAE.

QAE is the algorithm to estimate a probability amplitude of a marked state in a superposition. Consider the system consisting of some qubits. We set the system to the initial state where all qubits are set to $|0\rangle$ and write such a state as $|0\rangle$ for simplicity. Then, we assume that there exists a unitary transformation A on the system such that

$$A|0\rangle = a|\Psi\rangle + \sqrt{1-a^2}|\Psi_\perp\rangle, \quad (17)$$

where $|\Psi\rangle$ is the “marked state,” $|\Psi_\perp\rangle$ is a state orthogonal to $|\Psi\rangle$, and $0 < a < 1$. Typically, $|\Psi\rangle$ and $|\Psi_\perp\rangle$ are the states where a specific qubit takes $|1\rangle$ and $|0\rangle$, respectively. In addition to A , we use the following unitary operators S_0 and S_Ψ , which are defined as

$$S_0|\phi\rangle = \begin{cases} -|0\rangle & \text{if } |\phi\rangle = |0\rangle, \\ |\phi\rangle & \text{if } |\phi\rangle \text{ is orthogonal to } |0\rangle, \end{cases} \quad (18)$$

$$S_\Psi|\phi\rangle = \begin{cases} -|\Psi\rangle & \text{if } |\phi\rangle = |\Psi\rangle, \\ |\phi\rangle & \text{if } |\phi\rangle \text{ is orthogonal to } |\Psi\rangle. \end{cases} \quad (19)$$

S_0 can be constructed using a multicontrolled Toffoli gate, and S_Ψ is simply a controlled-Z gate if $|\Psi\rangle$ is defined as the state where a specific qubit is $|1\rangle$. Then, defining

$$Q := -AS_0A^{-1}S_\Psi, \quad (20)$$

we can construct a quantum algorithm (see [14] for details), which makes

$$O\left(\frac{1}{\epsilon}\right) \quad (21)$$

uses of Q [therefore, $O(1/\epsilon)$ uses of A] and outputs an estimate of a with an ϵ -additive error.

We make a comment here on success probability. In the algorithm of QAE [14], the success probability, that is, the probability that the algorithm outputs the estimation with the desired additive error, is not 1 but lower-bounded by $8/\pi^2$. However, we can enhance the success probability to an arbitrary level $1 - \gamma$, where $\gamma \in (0, 1)$, by repeating QAE $O(\ln(\gamma^{-1}))$ times. That is, taking the median of the results in the $O(\ln(\gamma^{-1}))$ runs of QAE, we can obtain the estimation with the additive error ϵ with probability $1 - \gamma$ [21,23]. Considering this point, we can write the number of calls to A in repeating QAE with an ϵ -additive error and a success probability larger than $1 - \gamma$ as

$$O\left(\frac{\ln(\gamma^{-1})}{\epsilon}\right). \quad (22)$$

If we set $1 - \gamma$ to some fixed value, say 99%, (22) is reduced to (21).

B. Assumptions

Next, we present some assumptions that are necessary for the method. The first one is as follows:

Assumption 1. The following oracles P_x and P_y are available:

$$P_x : |i\rangle |k\rangle |0\rangle \mapsto |i\rangle |k\rangle |x_k^{(i)}\rangle, \quad (23)$$

$$P_y : |k\rangle |0\rangle \mapsto |k\rangle |y_k\rangle \quad (24)$$

for any $i \in \{1, \dots, d\}$ and $k \in \{1, \dots, N_D\}$.

Here and hereafter, for a number x , the ket $|x\rangle$ corresponds to a computational basis state on a quantum register where the bit string represents the binary representation of x . Equations (23) and (24) mean that P_x and P_y output the element of X and $\tilde{y}$, respectively, for the specified index. Previous papers [1–6, 9, 24] also assume such oracles. We can construct P_x and P_y if quantum random access memories (QRAMs) [25] are available.

The second assumption is just a reproduction.

Assumption 2. X defined as (9) is full-rank.

Because of this, $\kappa(X)$, the condition number of X , can be defined, and W defined as (13) is invertible. Hereafter, we simply write $\kappa(X)$ as κ .

The third assumption is as follows:

Assumption 3.

$$0 \leq x_k^{(i)} \leq 1, 0 \leq y_k \leq 1 \quad (25)$$

for any $i \in \{1, \dots, d\}$ and $k \in \{1, \dots, N_D\}$.

That is, we assume that the explanatory variables and the objective variable are bounded by 0 and 1. Besides, we make the fourth assumption as follows:

Assumption 4. There is a positive number c (say, $\frac{1}{2}$), which is independent of N_D , ϵ , κ , and d , such that

$$\forall i \in \{1, \dots, d\}, w_{ii} = \frac{1}{N_D} \sum_{k=1}^{N_D} (x_k^{(i)})^2 > c. \quad (26)$$

Since $w_{ii} \leq 1$ is immediately derived from Assumption 3, Assumption 4 means that $c < w_{ii} \leq 1$.

Although Assumptions 3 and 4 are too strong seemingly, they should be assumed for successful regression, in either the classical or the quantum way, for the following reasons. First, we note that Assumption 3 is satisfied if we know the bounds for $x_k^{(i)}$ and y_k in advance and can rescale them. That is, for $i \in \{1, \dots, d\}$, although in general $x_k^{(i)}$'s are not in $[0, 1]$, we can redefine

$$\tilde{x}_k^{(i)} := \frac{x_k^{(i)} - L_i}{U_i - L_i} \quad (27)$$

as $x_k^{(i)}$ if we know L_i, U_i such that

$$\forall k \in \{1, \dots, N_D\}, L_i \leq x_k^{(i)} \leq U_i. \quad (28)$$

Then, redefined $x_k^{(i)}$'s are in $[0, 1]$. Similarly, redefining

$$\tilde{y}_k := \frac{y_k - L_y}{U_y - L_y} \quad (29)$$

as y_k with L_y, U_y such that

$$\forall k \in \{1, \dots, N_D\}, L_y \leq y_k \leq U_y \quad (30)$$

leads to $0 \leq y_k \leq 1$. Assumption 3 is then satisfied. Besides, if we know the bounds which are not too far from the typical scale of the original $x_k^{(i)}$'s, that is, if we can take L_i, U_i such

that $|L_i| \sim |U_i| \sim |x_k^{(i)}|$ for most k 's, Assumption 4 is satisfied. In summary, Assumptions 3 and 4 are naturally satisfied if we know the typical scales of $x_k^{(i)}$'s and y_k 's. Practically, we *must* know the typical scales, since we have to address the problem of *outliers*. Datasets often contain points whose explanatory and/or objective variables are much larger than those of others, because of various reasons (for example, misrecord). Such points are called outliers. It is widely known that outliers lead to inaccurate regression and so we have to address them. Typically, we omit them from data points used for regression or replace the values of the explanatory and/or objective variables out of some range with the upper or lower bound of the range. For such a preprocess, we have to know the typical scales of the variables. In fact, the previous paper [3] makes assumptions similar to Assumptions 3 and 4. Mentioning the necessity of preprocessing outliers, it assumes that the design matrix and the objective variable vector do not contain the extraordinarily large elements.

C. Details of our method

We now explain our method in detail. First, we present a lemma on the error in the solution of a system of linear equations where coefficients and constant terms contain errors.

Lemma 1. Let Assumptions 2–4 be satisfied. For given symmetric $\hat{W} \in \mathbb{R}^{d \times d}$ and $\tilde{\tilde{z}} \in \mathbb{R}^d$, consider a system of linear equations

$$\hat{W} \tilde{\tilde{a}} = \tilde{\tilde{z}}, \quad (31)$$

where $\tilde{\tilde{a}} \in \mathbb{R}^d$. For a given $\epsilon > 0$, if each element of $\delta W := \hat{W} - W$ and $\delta \tilde{\tilde{z}} := \tilde{\tilde{z}} - \tilde{z}$ has an absolute value smaller than ϵ' such that

$$\epsilon' < \min \left\{ \frac{c}{d\kappa^2}, \frac{c^2\epsilon}{2d^{3/2}\kappa^4} \right\}, \quad (32)$$

then $\tilde{\tilde{a}}$ is uniquely determined by solving Eq. (31), i.e., $\tilde{\tilde{a}} = \hat{W}^{-1}\tilde{\tilde{z}}$, and it becomes an $O(\epsilon)$ -additive approximation of $\tilde{a}$, which means that

$$\|\tilde{\tilde{a}} - \tilde{a}\|_\infty = O(\epsilon). \quad (33)$$

The proof is given in Appendix A 1. This lemma means that, if we want a solution of a system of linear equations with an $O(\epsilon)$ -additive error, it is sufficient to calculate coefficients and constant terms with an additive error ϵ' satisfying (32).

We therefore propose the following method for linear regression: we first estimate W in (13) and $\tilde{z}$ in (15) by a quantum method with ϵ' -additive error and then calculate (16) by some classical method. Since classical methods basically introduce no additional error, we can obtain a solution with $O(\epsilon)$ -additive error.

Then, we state a theorem on the complexity of our method, presenting the concrete procedure in the proof.

Theorem 1. Given $\epsilon > 0$, accesses to oracles P_x and P_y which satisfy Assumption 1, and $\{x_k^{(i)}\}_{i=1, \dots, d, k=1, \dots, N_D}$ and $\{y_k\}_{k=1, \dots, N_D}$

which satisfy Assumptions 2–4, there is a quantum algorithm that makes

$$O\left(\max \left\{ \frac{d^{3/2}\kappa^4}{\epsilon}, d\kappa^2 \right\} \times d^2 \ln(d)\right) \quad (34)$$

uses of P_x and

$$O\left(\max\left\{\frac{d^{3/2}\kappa^4}{\epsilon}, d\kappa^2\right\} \times d \ln(d)\right) \quad (35)$$

uses of P_y and, with a probability larger than 99%, outputs an $O(\epsilon)$ -additive approximation of $\bar{a}$, which is defined as (16).

Proof. The outline of the algorithm is as follows:

(1) Estimate the elements of W and $\bar{z}$ in (16) using a quantum algorithm based on QAE. Let the matrix and the vector consisting of the estimation results be $\hat{W}$ and $\hat{\bar{z}}$.

(2) Solve $\hat{W}\bar{a} = \hat{\bar{z}}$ by some classical solver of systems of linear equations (for example, row reduction). Let the solution be $\tilde{a}$. This is an output of our algorithm.

Since we do not use the oracles P_x, P_y in the second step, we focus on step (1). As we explained in Sec. III A, we can obtain an estimation $\hat{w}_{ij}$ of w_{ij} by QAE if we construct the following operators A_{ij} . A_{ij} transforms $|0\rangle$, a state in which all qubits are 0, to a state in the form of

$$\sqrt{w_{ij}}|\psi\rangle + \sqrt{1-w_{ij}}|\psi_\perp\rangle, \quad (36)$$

where $|\psi\rangle$ and $|\psi_\perp\rangle$ are some orthogonal states. Such an operator is constructed as follows:

(i) Prepare quantum registers $R_1, \dots, R_5$, which have enough qubits, and a single-qubit register R_6 . Set R_1, R_2 and the others to $|i\rangle, |j\rangle$, and $|0\rangle$, respectively.

(ii) Create $\frac{1}{\sqrt{N_D}} \sum_{k=1}^{N_D} |k\rangle$, that is, an equiprobable superposition of $|1\rangle, \dots, |N_D\rangle$ on R_3 .

(iii) Apply P_x to a block of R_1, R_3 , and R_4 , which outputs $x_k^{(i)}$ on R_4 . Similarly, apply P_x to a block of R_2, R_3 , and R_5 , which outputs $x_k^{(j)}$ on R_5 .

(iv) Using $x_k^{(i)}$ on R_4 and $x_k^{(j)}$ on R_5 , transform R_6 from $|0\rangle$ to $(\sqrt{1-x_k^{(i)}x_k^{(j)}}|0\rangle + \sqrt{x_k^{(i)}x_k^{(j)}}|1\rangle)$ by some arithmetic circuits and controlled rotations.⁵ Then, the resultant state is in the form of (36).

⁵More concretely, we can perform the following calculation:

$$\begin{aligned} & |x_k^{(i)}\rangle |x_k^{(j)}\rangle |0\rangle |0\rangle |0\rangle \\ \rightarrow & |x_k^{(i)}\rangle |x_k^{(j)}\rangle |x_k^{(i)}x_k^{(j)}\rangle |0\rangle |0\rangle \\ \rightarrow & |x_k^{(i)}\rangle |x_k^{(j)}\rangle |x_k^{(i)}x_k^{(j)}\rangle |\sqrt{x_k^{(i)}x_k^{(j)}}\rangle |0\rangle \\ \rightarrow & |x_k^{(i)}\rangle |x_k^{(j)}\rangle |x_k^{(i)}x_k^{(j)}\rangle |\sqrt{x_k^{(i)}x_k^{(j)}}\rangle (\sqrt{1-x_k^{(i)}x_k^{(j)}}|0\rangle + \sqrt{x_k^{(i)}x_k^{(j)}}|1\rangle), \end{aligned}$$

where the first, second, and last kets correspond to R_4, R_5 , and R_6 , respectively, and the third and fourth kets correspond to two ancillary registers, which are not displayed in (37). We used the multiplication circuit (e.g., [26]) at the first arrow, the circuit for the square root (e.g., [27]) at the second arrow, and the rotation gate on R_6 controlled by the second ancillary register at the last arrow.

Through steps (i)–(iv), the state is transformed as follows:

$$\begin{aligned} & |i\rangle |j\rangle |0\rangle |0\rangle |0\rangle |0\rangle \\ \xrightarrow{(ii)} & |i\rangle |j\rangle \left(\frac{1}{\sqrt{N_D}} \sum_{k=0}^{N_D} |k\rangle\right) |0\rangle |0\rangle |0\rangle \\ \xrightarrow{(iii)} & |i\rangle |j\rangle \left(\frac{1}{\sqrt{N_D}} \sum_{k=0}^{N_D} |k\rangle |x_k^{(i)}\rangle |x_k^{(j)}\rangle\right) |0\rangle \\ \xrightarrow{(iv)} & |i\rangle |j\rangle \left[\frac{1}{\sqrt{N_D}} \sum_{k=0}^{N_D} |k\rangle |x_k^{(i)}\rangle |x_k^{(j)}\rangle \right. \\ & \left. \otimes \left(\sqrt{1-x_k^{(i)}x_k^{(j)}}|0\rangle + \sqrt{x_k^{(i)}x_k^{(j)}}|1\rangle\right)\right]. \quad (37) \end{aligned}$$

To estimate w_{ij} with an additive error ϵ' , QAE makes $O(\frac{1}{\epsilon'})$ uses of A_{ij} . In the current case, A_{ij} contains $O(1)$ uses of P_x (precisely, two uses). In total, we use it $O(\frac{1}{\epsilon'})$ times in the whole process of the QAE. We can obtain an estimation $\hat{z}_i$ of z_i in the similar way by replacing one of two P_x 's with P_y and $x_k^{(j)}$ with y_k .

As shown in Lemma 1, in order to obtain an ϵ -additive approximation of $\bar{a}$, it is sufficient to take ϵ' satisfying (32). Therefore, the number of calling P_x, P_y in one QAE for w_{ij} or z_i is

$$O\left(\max\left\{\frac{d^{3/2}\kappa^4}{\epsilon}, d\kappa^2\right\}\right). \quad (38)$$

Here, we omit c since it is independent of N_D, κ, d (Assumption 4) and of course ϵ .

Then, let us recall the issue of the success probability, which is mentioned in Sec. III A. Since the numbers of w_{ij} 's and z_i 's are $d(d+1)/2$ and d , respectively, in order to successfully estimate all of them with a probability larger than $0.99 = 1 - 0.01$, it suffices to make the success probability of each estimation larger than $1 - \frac{0.01}{d^2}$. Therefore, it is sufficient to repeat QAE $O(\ln(\frac{d^2}{0.01})) = O(\ln(d))$ times in estimating one of w_{ij} 's or z_i 's. Combining this point and (38), and noting the numbers of w_{ij} 's and z_i 's, we see that the total number of calls to P_x and P_y in the whole algorithm are (34) and (35), respectively.

D. Time complexity

Here, let us make some comments on overall *time complexity*. Although we saw that we can reduce the *query complexity*, that is, the number of calls to P_x and P_y , exponentially with respect to N_D compared to the naive classical method, the time for one such query might depend on N_D . Fortunately, in the following examples, the time complexity of one query is at most logarithmic with respect to N_D , which means that our method provides speed-up also in time complexity.

We first consider LSM, where the explanatory and objective variables are not given as exogenous data, but are produced by a simulation. Concretely, P_x is the oracle to generate sample paths of time evolution of asset prices, P_y is the oracle to calculate the cash flows on paths, and N_D is the number of the paths. Typically, we generate asset price paths based on some stochastic differential equation, using random

numbers. The implementation of such a calculation as a quantum circuit has already been considered [28–30]. In such a circuit, we create and use random numbers with $O(\ln(N_D))$ digits in order to generate N_D different paths. The gate number for creating such numbers and arithmetic operations on them is $O(\text{polylog}(N_D))$, and so is the time complexity. We can summarize this situation as follows: we aim to approximate some complex function by linear regression, and the quantum circuits which calculate the explanatory and objective variables with $O(\text{polylog}(N_D))$ time complexity are available. We expect that this is not unique to LSM.

Next, let us consider the cases where we use a QRAM to implement the oracles. According to [25], once we are given the QRAM containing N_D data points, we can load them into a register with $O(\text{polylog}(N_D))$ time complexity per query. Thus, the cost of querying the oracle is negligible. However, preparing such a QRAM also takes time, which must be taken into account. The reasonable assumption is that we are initially given the data points as classical data, and load them into the QRAM, which takes $O(N_D)$ time complexity. Even if we consider the QRAM initialization time, in practical uses of linear regression, our quantum method can provide a reduction of time complexity in the entire process of data analysis. For example, consider the situation where we explore an optimal combination of preprocessing, such as one-hot encoding and logarithmic transformation, by trial and error. Such transformations, by which we aim to enhance explanatory power of the variables, are ubiquitous in data analysis, and we often repeat regression for one data set applying various patterns of transformation and compare the results. In this situation, the costliest part of the total calculation is a series of classical regression in many trials for the classical method, but a single QRAM initialization at the very beginning for the our method, which will be less time-consuming. Therefore, we conclude that the proposed method is totally faster than the naive classical method.

IV. EXTENSION TO A CLASS OF CONVEX OPTIMIZATION

A. Linear regression as optimization by Newton's method

In this section, we extend our method for linear regression to more general optimization problems. Before this, we first present another interpretation of (11), the formula for the solution of linear regression. We regard linear regression as an optimization problem of

$$F(\vec{a}) = \frac{1}{2N_D} \|\vec{y} - X\vec{a}\|^2 = \frac{1}{2N_D} \sum_{k=1}^{N_D} \left(\sum_{i=1}^d a_i x_k^{(i)} - y_k \right)^2. \quad (39)$$

This can be rewritten as

$$F(\vec{a}) = \frac{1}{N_D} \sum_{k=1}^{N_D} f(\vec{a}; \vec{x}_k, y_k), \quad (40)$$

where

$$f(\vec{a}; \vec{x}_k, y_k) = \frac{1}{2} \left(\sum_{i=1}^d a_i x_k^{(i)} - y_k \right)^2. \quad (41)$$

The first and second derivatives of F are

$$\begin{aligned} \frac{\partial}{\partial a_i} F(\vec{a}) &= \frac{1}{N_D} \sum_{k=1}^{N_D} \frac{\partial}{\partial a_i} f(\vec{a}; \vec{x}_k, y_k) \\ &= \frac{1}{N_D} \sum_{k=1}^{N_D} x_k^{(i)} \left(\sum_{j=1}^d a_j x_k^{(j)} - y_k \right), \end{aligned} \quad (42)$$

$$\frac{\partial^2}{\partial a_i \partial a_j} F(\vec{a}) = \frac{1}{N_D} \sum_{k=1}^{N_D} \frac{\partial^2}{\partial a_i \partial a_j} f(\vec{a}; \vec{x}_k, y_k) = \frac{1}{N_D} \sum_{k=1}^{N_D} x_k^{(i)} x_k^{(j)}, \quad (43)$$

respectively. This means that $W = \frac{1}{N_D} X^T X$ and $-\vec{z} = -\frac{1}{N_D} X^T \vec{y}$ are the Hessian matrix and the gradient vector of F at $\vec{a} = \vec{0}$, respectively. Besides, the updating formula in Newton's method is

$$\vec{a}_{n+1} = \vec{a}_n - H_F^{-1}(\vec{a}_n) \vec{g}_F(\vec{a}_n), \quad (44)$$

where H_F and $\vec{g}_F$ are the Hessian and the gradient of the function F , respectively, and $\vec{a}_n$ is the optimization variable after the n th update. Then, we can interpret (11) as a one-time update in Newton's method from the initial point $\vec{a}_0 = \vec{0}$. Note that Newton's method gives the exact solution by only one update from any initial point, if the objective function is quadratic.

In summary, we can consider our method as optimization of the objective function (39) by Newton's method, where calculation of the gradient and the Hessian, which is time-consuming in the classical method, is done by the QAE-based method.

B. Extension of our method: The QAE-based Newton's method

On the basis of the above discussion, it is now straightforward to extend our method to a more general class of optimization problems. That is, keeping the updating formula (44), we can perform Newton's method based on the gradient and the Hessian estimated by QAE.

Concretely, we consider an optimization problem in which the objective function can be written as a sum of the values of some function with different inputs:

$$F(\vec{a}) = \frac{1}{N_D} \sum_{k=1}^{N_D} f(\vec{a}, \vec{c}_k). \quad (45)$$

Here, f is the real-valued twice-differentiable function, which are shared by all the terms. Its inputs are the optimization variables $\vec{a} \in \mathbb{R}^d$ and some parameters $\vec{c}_k$, which are different in each term. Some conditions on F necessary for convergence analysis are given in Sec. IV C. It is obvious that the objective functions (39) fall into (45). For the objective function like (45), the gradient $\vec{g}_F(\vec{a}) = (g_{F,1}(\vec{a}), \dots, g_{F,d}(\vec{a}))^T$ and the Hessian $H_F(\vec{a}) = (h_{F,ij}(\vec{a}))_{1 \leq i \leq d, 1 \leq j \leq d}$ are given as

$$g_{F,i}(\vec{a}) = \frac{\partial}{\partial a_i} F(\vec{a}) = \frac{1}{N_D} \sum_{k=1}^{N_D} f_i(\vec{a}, \vec{c}_k), \quad (46)$$

$$h_{F,ij}(\vec{a}) = \frac{\partial^2}{\partial a_i \partial a_j} F(\vec{a}) = \frac{1}{N_D} \sum_{k=1}^{N_D} f_{ij}(\vec{a}, \vec{c}_k), \quad (47)$$

where we simply write $\frac{\partial}{\partial a_i} f$ and $\frac{\partial^2}{\partial a_i \partial a_j} f$ as f_i and f_{ij} , respectively.

Then, we estimate the gradient and the Hessian as follows. We assume the availability of the following:

(i) P_c , which outputs $\vec{c}_k$ for given k :

$$P_c : |k\rangle |0\rangle \mapsto |k\rangle |\vec{c}_k\rangle. \quad (48)$$

This can be constructed by QRAM.

(ii) P_i for $i = 1, \dots, d$, which outputs $f_i(\vec{a}, \vec{c}_k)$ for given $\vec{a}$ and $\vec{c}_k$:

$$P_i : |\vec{a}\rangle |\vec{c}_k\rangle |0\rangle \mapsto |\vec{a}\rangle |\vec{c}_k\rangle |f_i(\vec{a}, \vec{c}_k)\rangle. \quad (49)$$

(iii) P_{ij} for $i, j = 1, \dots, d$, which outputs $f_{ij}(\vec{a}, \vec{c}_k)$ for given $\vec{a}$ and $\vec{c}_k$:

$$P_{ij} : |\vec{a}\rangle |\vec{c}_k\rangle |0\rangle \mapsto |\vec{a}\rangle |\vec{c}_k\rangle |f_{ij}(\vec{a}, \vec{c}_k)\rangle. \quad (50)$$

Then, preparing appropriate registers, we can perform the following computation:

$$\begin{aligned} & |\vec{a}\rangle |0\rangle |0\rangle |0\rangle |0\rangle \\ & \rightarrow \left(\frac{1}{\sqrt{N_D}} \sum_{k=0}^{N_D} |\vec{a}\rangle |k\rangle \right) |0\rangle |0\rangle |0\rangle \\ & \rightarrow \left(\frac{1}{\sqrt{N_D}} \sum_{k=0}^{N_D} |\vec{a}\rangle |k\rangle |\vec{c}_k\rangle \right) |0\rangle |0\rangle \\ & \rightarrow \left(\frac{1}{\sqrt{N_D}} \sum_{k=0}^{N_D} |\vec{a}\rangle |k\rangle |\vec{c}_k\rangle |f_i(\vec{a}; \vec{c}_k)\rangle \right) |0\rangle \\ & \rightarrow \frac{1}{\sqrt{N_D}} \sum_{k=0}^{N_D} |\vec{a}\rangle |k\rangle |\vec{c}_k\rangle |f_i(\vec{a}; \vec{c}_k)\rangle \\ & \otimes (\sqrt{1 - f_i(\vec{a}; \vec{c}_k)} |0\rangle + \sqrt{f_i(\vec{a}; \vec{c}_k)} |1\rangle), \end{aligned} \quad (51)$$

where P_c and P_i are used at the second and third arrows, respectively. We then obtain an estimation of $g_i(\vec{a})$ by estimating the probability that the last qubit takes 1 by QAE. We can also estimate $h_{ij}(\vec{a})$ similarly, replacing P_i with P_{ij} and $f_i(\vec{a}, \vec{c}_k)$ with $f_{ij}(\vec{a}, \vec{c}_k)$. Again, in order to estimate one $g_i(\vec{a})$ or $h_{ij}(\vec{a})$ with ϵ -additive error, the number of calling P_i and P_{ij} is at most $O(1/\epsilon)$, which means the exponential speedup with respect to N_D compared with classical iterative calculation.

Using the gradient and the Hessian estimated as above, we update $\vec{a}_n$ to $\vec{a}_{n+1}$ similarly to (44), that is,

$$\vec{a}_{n+1} = \vec{a}_n - \hat{H}_F^{-1}(\vec{a}_n) \vec{g}_F(\vec{a}_n), \quad (52)$$

where $\vec{g}_F(\vec{a}_n)$ and $\hat{H}_F(\vec{a}_n)$ are the estimated gradient and Hessian, respectively. After sufficiently many iterations, we obtain the approximated solution of the optimization. Hereafter, we call this method the *QAE-based Newton's method*.

Note that $\hat{H}_F(\vec{a}_n)$ must be invertible so that the update (52) can be defined. Hereafter, we consider the situation where the original Hessian $H_F(\vec{a}_n)$ is positive-definite and therefore invertible. To keep such a property, we have to obtain $\hat{H}_F(\vec{a}_n)$ accurately enough.

C. Convergence analysis of the QAE-based Newton's method

Let us estimate the complexity of the QAE-based Newton's method to obtain an approximated solution with ϵ -additive error. For a mathematically rigorous discussion, we first make some assumptions on the objective function $F : \mathbb{R}^d \rightarrow \mathbb{R}$.

Assumption 5. F is twice-differentiable.

This is reproduced since we assumed that f in (45) is twice-differentiable.

Assumption 6. F is μ -strongly convex, that is, there exists a positive number μ such that

$$\forall \vec{a}, \vec{b} \in \mathbb{R}^d, F(\vec{a}) \geq F(\vec{b}) + \vec{g}_F(\vec{b}) \cdot (\vec{a} - \vec{b}) + \frac{\mu}{2} \|\vec{a} - \vec{b}\|^2. \quad (53)$$

This assumption means that the eigenvalues of $H_F(\vec{a})$ are greater than or equal to μ for any $\vec{a} \in \mathbb{R}^d$, that is,

$$\forall \vec{a} \in \mathbb{R}^d, H_F(\vec{a}) \succeq \mu I_d, \quad (54)$$

where I_d is the $d \times d$ identity matrix and for $A, B \in \mathbb{R}^d$, $A \succeq B$ means that $A - B$ is positive-semidefinite. This immediately leads to

$$\forall \vec{a} \in \mathbb{R}^d, \|(H_F(\vec{a}))^{-1}\| \leq \frac{1}{\mu}. \quad (55)$$

Assumption 7. F has an M -Lipschitz Hessian, that is,

$$\forall \vec{a}, \vec{b} \in \mathbb{R}^d, \|H_F(\vec{a}) - H_F(\vec{b})\| \leq M \|\vec{a} - \vec{b}\|. \quad (56)$$

This assumption leads to the following inequality:

$$\forall \vec{a}, \vec{b} \in \mathbb{R}^d, \|\vec{g}_F(\vec{a}) - \vec{g}_F(\vec{b}) - H_F(\vec{b})(\vec{a} - \vec{b})\| \leq \frac{M}{2} \|\vec{a} - \vec{b}\|^2. \quad (57)$$

Assumptions 5–7 are usually made in the discussion on convergence properties of the *ordinary* Newton's method, that is, cases where the gradient and the Hessian can be exactly computed in the classical way (see, for example, [31]). We do not make any additional assumptions for the QAE-based Newton's method.

Next, let us define some quantities. Since QAE introduces errors in the estimated Hessian and gradient, we have to consider Newton's method in which the update difference contains some error. For $\vec{a} \in \mathbb{R}^d$, we define $\vec{\Delta}_F(\vec{a})$ as

$$\vec{\Delta}_F(\vec{a}) := [\hat{H}_F(\vec{a})]^{-1} \vec{g}_F(\vec{a}) - [H_F(\vec{a})]^{-1} \vec{g}_F(\vec{a}). \quad (58)$$

Besides, we write the minimum⁶ that we search as $\vec{a}^* := \arg\min_{\vec{a} \in \mathbb{R}^d} F(\vec{a})$, the optimization variable after the n th update as $\vec{a}_n$, and the difference between $\vec{a}^*$ and $\vec{a}_n$ as $\delta_n := \|\vec{a}_n - \vec{a}^*\|$.

Then, we can show the following lemma, which is repeatedly used.

Lemma 2. Let Assumptions 5–7 be satisfied. Then, for any non-negative number ϵ and any $\vec{a} \in \mathbb{R}^d$ such that

$$\|\vec{\Delta}_F(\vec{a})\| \leq \epsilon, \quad (59)$$

⁶Since we are considering the convex optimization as stated in Assumption 6, there is only one global minimum.

the following inequality holds:

$$\delta' \leq \frac{M}{2\mu} \delta^2 + \epsilon, \quad (60)$$

where $\delta := \|\bar{a} - \bar{a}^*\|$, $\delta' := \|\bar{a}' - \bar{a}^*\|$, and $\bar{a}' = \bar{a} - [\hat{H}_F(\bar{a})]^{-1} \hat{g}_F(\bar{a})$. Furthermore, when

$$\frac{2M}{\mu} \epsilon < 1 \quad (61)$$

is satisfied, the following holds:

$$\begin{aligned} \delta' &< \delta & \text{if } \delta_- < \delta < \delta_+, \\ \delta' &\leq \delta_- & \text{if } \delta \leq \delta_-, \end{aligned} \quad (62)$$

where

$$\delta_{\pm} := \frac{\mu}{M} \left(1 \pm \sqrt{1 - \frac{2M}{\mu} \epsilon} \right). \quad (63)$$

The proof is given in Appendix A 2. Here, let us comment on what Lemma 2 implies. Equation (60) indicates that, even when the update differences in Newton's method contain errors at most ϵ , the difference δ between the optimization variables $\bar{a}$ and the optimal point $\bar{a}^*$ quadratically converges like Newton's method with no error, as long as $\epsilon \lesssim \frac{M}{2\mu} \delta^2$. More strictly, while $\delta_- < \delta$, δ decreases at every update, as shown in (62). On the other hand, after δ reaches δ_- , ϵ is not negligible in (60), and therefore δ does not necessarily decrease. Nevertheless, δ does not exceed δ_- once it goes below. Since $\delta_- < 2\epsilon$, we can make $\bar{a}$ converge with desired accuracy if we can suppress ϵ .

Using Lemma 2, we obtain the following lemma, which shows how many updates are sufficient for δ to reach 2ϵ in Newton's method with erroneous update differences.

Lemma 3. Let Assumptions 5–7 be satisfied. Suppose that we repeatedly update $\bar{a} \in \mathbb{R}^d$ by (52) from some initial point $\bar{a}_0$, where we write the result of n -times updates as $\bar{a}_n$ and define $\delta_n := \|\bar{a}_n - \bar{a}^*\|$ for $n = 0, 1, 2, \dots$. Then, for any positive number ϵ satisfying (61) and any $\bar{a}_0$ such that

$$\|\bar{a}_0 - \bar{a}^*\| < \frac{\mu}{M}, \quad (64)$$

if (59) holds for $\bar{a} = \bar{a}_n$, $n = 0, 1, 2, \dots$, there exists a non-negative integer n_{it} such that

$$\delta_n \leq 2\epsilon \quad (65)$$

for any $n \geq n_{\text{it}}$, where

$$n_{\text{it}} := \max \left\{ \left\lceil \log_2 \left(\frac{\ln \left(\frac{2M\epsilon}{\mu} \right)}{2 \ln \left(\frac{M\delta_0}{\mu} \right)} \right) \right\rceil + 1, 1 \right\}. \quad (66)$$

The proof is given in Appendix A 3.

Next, we consider how accurate we should estimate the gradient and the Hessian in order to suppress the error in the update difference to the order of ϵ .

Lemma 4. Let Assumptions 5–7 be satisfied. Besides, suppose that we are given a positive integer n , a positive number ϵ satisfying (61), and $\bar{a} \in \mathbb{R}^d$ satisfying $\delta < \frac{2\mu}{M}$, where $\delta := \|\bar{a} - \bar{a}^*\|$. Then, in order for $\Delta_F(\bar{a})$ defined as (58) to satisfy $\|\bar{\Delta}_F(\bar{a})\| \leq \epsilon$, it is sufficient that each component of the estimated gradient $\hat{g}_F(\bar{a})$ and Hessian $\hat{H}_F(\bar{a})$ has an additive error

ϵ'_g and ϵ'_H such that

$$\epsilon'_g \leq \frac{\mu\epsilon}{2d^{1/2}} \quad (67)$$

and

$$\epsilon'_H \leq \frac{\mu\epsilon}{4\tilde{\delta}d}, \quad (68)$$

where $\tilde{\delta} := \max\{\delta, \delta_-\}$, respectively.

Lemma 5. Let Assumptions 5–7 be satisfied. Besides, suppose that we are given a positive number ϵ satisfying (61) and an initial point $\bar{a}_0 \in \mathbb{R}^d$ satisfying $\delta_0 := \|\bar{a}_0 - \bar{a}^*\| < \delta_+$. Furthermore, let $\bar{a}_n \in \mathbb{R}^d$ be a vector given by n -times updates by (52) from the initial point $\bar{a}_0$. Then, $\Delta_F(\bar{a}_n)$ defined as (58) satisfies

$$\|\Delta_F(\bar{a}_n)\| \leq \epsilon \quad (69)$$

for any positive integer n , if each component of $\hat{g}_F(\bar{a})$ and $\hat{H}_F(\bar{a})$ has an additive error ϵ'_g and ϵ'_H satisfying (67) and

$$\epsilon'_H \leq \frac{\mu\epsilon}{4\tilde{\delta}_0d}, \quad (70)$$

where $\tilde{\delta}_0 := \max\{\delta_0, \delta_-\}$, respectively.

The proofs of Lemmas 4 and 5 are given in Appendixes A 4 and A 5, respectively.

Combining Lemma 3 and Lemma 5, we immediately obtain the following theorem:

Theorem 2. Let Assumptions 5–7 be satisfied. Besides, suppose that we are given a positive number ϵ satisfying (61) and $\bar{a}_0$ satisfying (64). Then, using the QAE-based Newton's method, which is based on the updating formula (52), we obtain a 2ϵ -additive approximation of $\bar{a}^*$ by n_{it} -times updates, where n_{it} is given by (66), with a success probability higher than 99%. In the process, the total number of calls P_i , $i = 1, \dots, d$, is

$$N_{\text{1stDer}} = O\left(\frac{d^{3/2}}{\mu\epsilon} n_{\text{it}} \ln(n_{\text{it}} d^2)\right), \quad (71)$$

which for P_{ij} , $i, j = 1, \dots, d$, is

$$N_{\text{2ndDer}} = O\left(\frac{\tilde{\delta}_0 d^3}{\mu\epsilon} n_{\text{it}} \ln(n_{\text{it}} d^2)\right), \quad (72)$$

and that for P_c is

$$N_c = N_{\text{1stDer}} + N_{\text{2ndDer}}. \quad (73)$$

Proof. At first, let us consider a situation where all the estimation processes in the QAE-based Newton's method are successful, more concretely, all the estimations have errors smaller than the desired level. Correspondingly, suppose that, for ϵ'_g satisfying (67) and ϵ'_H satisfying (70), we can calculate each component of $\hat{g}_F$ and $\hat{H}_F$ with an ϵ'_g -additive error and an ϵ'_H -additive error, respectively, at each update in the QAE-based Newton's method. Because of Lemma 5, this means that (69) is satisfied at each update. Then, from Lemma 3, we obtain the optimization variable $\bar{a}_{n_{\text{it}}}$ satisfying (65), which is therefore 2ϵ -approximation of $\bar{a}^*$, after n_{it} -time updates.

Then, let us evaluate the total number of calls to P_i and $P_{i,j}$ in the above process, recalling that the success probability of QAE is not 1. We calculate the elements of $\hat{g}_F$ and $\hat{H}_F$,

whose number is $O(d^2)$ in total, at n_{it} updates. Therefore, the total number of such calculations is $O(n_{it}d^2)$. To make the probability that all calculations are done with required errors larger than 99%, it suffices to enhance the success probability of each calculation to $1 - \frac{0.01}{n_{it}d^2}$. This can be achieved by repeating QAEs $O(\ln(n_{it}d^2))$ times in each calculation. Besides, in one trial in repeating QAEs, it is sufficient to make $O(\frac{1}{\epsilon'_g})$ calls to P_i [$O(\frac{1}{\epsilon'_H})$ calls to $P_{i,j}$] in order to get an element of $\tilde{g}_F$ ($\tilde{H}_F$) with an ϵ'_g -additive (ϵ'_H -additive) error. In summary, we calculate the d components of $\tilde{g}_F$ by $O(\ln(n_{it}d^2))$ -time repeating QAEs with $O(\frac{1}{\epsilon'_g})$ calls to P_i at each of n_{it} updates, and therefore the total call number of P_i becomes (71). Similarly, that of $P_{i,j}$ becomes (72).

Since one call to P_i or $P_{i,j}$ accompanies one call to P_c , we obtain (73).

D. Newton's method based on classical Monte Carlo

The important feature of the QAE-based Newton's method is that we estimate the components in the Hessian and the gradient, which are represented as the sum of many similar terms, by QAE, or, more concretely, the procedure similar to the quantum algorithm for Monte Carlo integration based on QAE [15,21]. It is natural to compare the QAE-based Newton's method with the classical Monte Carlo (CMC) -based Newton's method, which is just Newton's method whose summation parts for calculating the Hessian and the gradient are replaced with CMC. If we can use the oracles similar to those in the above discussion, P_c , P_i , and $P_{i,j}$ in Sec. IV on a classical computer, we can estimate the components of the Hessian and the gradient also by CMC, that is, we can take the average of the values of sampled terms in the sum. Note that the classical counterpart of a QRAM, which can be used for P_x , P_y , and P_c , is just a RAM.

Let us estimate the complexity of this method. In the classical Monte Carlo, the estimation error is proportional to $N_{\text{samp}}^{-1/2}$, where N_{samp} is the sample number. More precisely, asymptotically, the deviation of the estimated value from the true value is less than $\frac{C}{\sqrt{N_{\text{samp}}}}$ with a probability $1 - \gamma$, where $C = O(\text{polylog}(\gamma))$. In other words, it is sufficient to take $O(\frac{\text{polylog}(\gamma)}{\epsilon^2})$ samples in order to obtain an estimation with error less than ϵ with probability higher than $1 - \gamma$. Besides, note that the number of calling for each oracle is proportional to the sample number. Then, by a discussion similar to that on Theorem 2, we see that we obtain a 2ϵ -additive approximation of $\tilde{a}^*$ by the CMC-based Newton's method with a probability higher than 99%. In the process, the iteration number n_{it} is given as (66), the total number of calling P_i , $i = 1, \dots, d$, is

$$N_{1\text{stDer}} = O\left(\frac{d^2}{\mu^2\epsilon^2} n_{it} \text{polylog}(n_{it}d^2)\right), \quad (74)$$

which for $P_{i,j}$, $i, j = 1, \dots, d$, is

$$N_{2\text{ndDer}} = O\left(\frac{(\tilde{\delta}_0)^2 d^4}{\mu^2\epsilon^2} n_{it} \text{polylog}(n_{it}d^2)\right), \quad (75)$$

and that for P_c is (73). Therefore, as the QAE-based Newton's method does, the CMC-based Newton's method removes the

dependency of the query complexity on N_D , even though it is classical. Note that the complexity of the QAE-based Newton's method is smaller than the CMC-based one, due to the so-called quadratic quantum speedup of Monte Carlo integration.

E. Related previous works

As a final comment, we briefly refer to some previous works [24,32], which used similar ideas to ours in the sense that the derivatives of the objective function are calculated by QAE. These papers considered not Newton's method but gradient descent and its application to an optimization problem with an objective function consisting of many similar terms, which is less general than (45) but includes linear regression. Then, they aimed at speedup of gradient calculation by QAE similarly to ours. Compared with Newton's method, gradient descent has both pros and cons. As pros, it requires not a Hessian but only a gradient, and it reaches the minimum from any initial point in convex optimization. On the other hand, as cons, it usually requires more iterations than Newton's method, and there is an issue on choice of appropriate step size.

V. SUMMARY

In this paper, we proposed a quantum algorithm for linear regression, or, more concretely, estimation of regression coefficients as classical data. Existing algorithms such as [1,3] create the quantum state encoding coefficients in its amplitude by the HHL algorithm [10] or its modification and then read out the coefficients. On the other hand, in our method, we estimate the elements of $W = \frac{1}{N_D} X^T X$ and $\tilde{z} = \frac{1}{N_D} X^T \tilde{y}$, where $X = (x_k^{(i)})_{\substack{1 \leq i \leq d \\ 1 \leq k \leq N_D}}$ is the design matrix, $\tilde{y} = (y_1, \dots, y_k)^T$ is

the objective variable vector, and N_D is the number of the data points, and then we find the coefficients by classical computation of $\tilde{a} = W^{-1} \tilde{z}$. Since, as shown in (13) and (15), the elements have the form of the sum of $x_k^{(i)} x_k^{(j)}$ or $x_k^{(i)} y_k$ over data points, we can estimate them by QAE [14–20], assuming availability of the oracles P_x and P_y which output $x_k^{(i)}$ and y_k , respectively, for specified i and k . The query complexity of our method is given as (34) and (35), which means exponential speedup with respect to N_D compared with the naive classical method, and improvement with respect to the tolerance error ϵ compared with the previous quantum methods such as [1,3].

Finally, we extended our method to more general optimization problems, that is, convex optimization with an objective function consisting of many similar terms like (45). In light of the interpretation of linear regression as Newton's method, we proposed the QAE-based Newton's method, in which the gradient and the Hessian are estimated by QAE. Introducing effects of estimation errors in the ordinary discussion on convergence of Newton's method, we derived the convergence property and the query complexity of the QAE-based Newton's method. Even if there are estimation errors, the method shows well-known quadratic convergence and reaches the solution in a small number of iterations.

Obtaining the improved dependence of complexity on ϵ , we expect that we can apply our method to mid-sized but oft-

repeated regression problems like LSM. Generally speaking, our method can be better than the previous quantum methods and the naive classical method when $d, \kappa \ll \frac{1}{\epsilon} \ll N_D$. On the other hand, since the complexity of our method depends on d and κ more strongly than the previous quantum methods, they will be better when $\frac{1}{\epsilon} \ll d$ or $\frac{1}{\epsilon} \ll \kappa$. Since the naive classical method does not induce any error as quantum ones, it will be better when $N_D \ll \frac{1}{\epsilon}$.

In future work, we will consider implementation of LSM on quantum computers using our method for linear regression, as a concrete and practical use case of quantum computing in financial industry.

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APPENDIX: PROOFS OF THE LEMMAS

1. Proof of Lemma 1

Proof. First, let us prove that $\hat{W}$ is invertible under

$$\epsilon' < c/d\kappa^2. \quad (\text{A1})$$

Note that W is positive-definite, and, according to discussions on perturbation on eigenvalues (see, for example, [33]),

$$|\hat{\lambda}_{\min} - \lambda_{\min}| \leq \|\delta W\|, \quad (\text{A2})$$

where $\lambda_{\min}$ and $\hat{\lambda}_{\min}$ are the smallest eigenvalues of W and $\hat{W}$, respectively. Therefore, it is sufficient to prove $\|\delta W\| < \lambda_{\min}$ in order to prove that $\hat{W}$ is positive-definite, and then invertible.

Then, let us bound $\lambda_{\min}$ first. Note that

$$\|W\| > c. \quad (\text{A3})$$

We can see this from

$$\|W\| \geq \frac{1}{d} \text{Tr} W \quad (\text{A4})$$

and

$$\text{Tr} W = \sum_{i=1}^d w_{ii} > dc, \quad (\text{A5})$$

where we used Assumption 4. Equation (A3) leads to the following inequality:

$$\lambda_{\min} > \frac{c}{\kappa^2}, \quad (\text{A6})$$

since

$$\lambda_{\min} = \frac{\lambda_{\max}}{\kappa(W)} = \frac{\|W\|}{\kappa^2}, \quad (\text{A7})$$

where $\lambda_{\max}$ is the largest eigenvalue of W and we used $\kappa(W) = \kappa^2 = \lambda_{\max}/\lambda_{\min}$ and $\|W\| = \lambda_{\max}$.

Next, let us consider $\|\delta W\|$. This can be upper bounded as follows:

$$\|\delta W\| < d\epsilon'. \quad (\text{A8})$$

This is because

$$\|\delta W\| \leq \|\delta W\|_F = \left(\sum_{i=1, \dots, d} \sum_{j=1, \dots, d} |\delta w_{ij}|^2 \right)^{1/2} < d\epsilon', \quad (\text{A9})$$

where the last inequality is satisfied due to the assumption $|\delta w_{ij}| < \epsilon'$.

Combining (A6) and (A8), we see that, for ϵ' satisfying (A1), $\|\delta W\| < \lambda_{\min}$ holds, and therefore $\hat{W}$ is invertible.

Then, let us prove (33). We use a well-known formula (see [22])

$$\frac{\|\tilde{a} - \bar{a}\|}{\|\bar{a}\|} \leq \kappa(W) \left(\frac{\|\delta W\|}{\|W\|} + \frac{\|\delta \tilde{z}\|}{\|\tilde{z}\|} \right) + O((\epsilon')^2). \quad (\text{A10})$$

This can be transformed as

$$\|\tilde{a} - \bar{a}\| \leq \kappa^4 \left(\frac{\|\tilde{z}\| \cdot \|\delta W\|}{\|W\|^2} + \frac{\|\delta \tilde{z}\|}{\|W\|} \right) + O((\epsilon')^2), \quad (\text{A11})$$

where we used

$$\|\bar{a}\| = \|W^{-1}\tilde{z}\| \leq \|W^{-1}\| \cdot \|\tilde{z}\| = \frac{\kappa(W)\|\tilde{z}\|}{\|W\|} \quad (\text{A12})$$

and $\kappa(W) = \kappa^2$.

Let us bound the terms in the parentheses on the right-hand side in (A11). To bound the first term, we need another inequalities:

$$\|\tilde{z}\| \leq \sqrt{d}, \quad (\text{A13})$$

which follows from

$$0 \leq z_i = \frac{1}{N_D} \sum_{k=1}^{N_D} x_k^{(i)} y_k \leq 1. \quad (\text{A14})$$

Combining (A3), (A8), and (A13), we obtain

$$\frac{\|\tilde{z}\| \cdot \|\delta W\|}{\|W\|^2} < \frac{d^{3/2}\epsilon'}{c^2}. \quad (\text{A15})$$

Next, let us consider the second term $\|\delta \tilde{z}\|/\|W\|$. This is bounded as

$$\frac{\|\delta \tilde{z}\|}{\|W\|} < \frac{\sqrt{d}\epsilon'}{c}. \quad (\text{A16})$$

Here, we used

$$\|\delta \tilde{z}\| \leq \sqrt{d}\epsilon', \quad (\text{A17})$$

which follows from the assumption $|\delta z_i| < \epsilon'$, and (A3).

Combining (A11), (A15), and (A16), we obtain

$$\begin{aligned} \|\tilde{a} - \bar{a}\| &\leq \kappa^4 \left(\frac{d^{3/2}\epsilon'}{c^2} + \frac{d^{1/2}\epsilon'}{c} \right) + O((\epsilon')^2) \leq \frac{2d^{3/2}\kappa^4}{c^2} \epsilon' \\ &\quad + O((\epsilon')^2), \end{aligned} \quad (\text{A18})$$

where the second inequality holds since $d \geq 1$ and $c \leq 1$. Noting that $\|\tilde{a} - \bar{a}\|_\infty \leq \|\tilde{a} - \bar{a}\|$, we finally obtain (33) for ϵ' satisfying $\epsilon' < c^2\epsilon/2d^{3/2}\kappa^4$.

2. Proof of Lemma 2

Proof. We can see that

$$\begin{aligned}
 \delta' &= \|\vec{a}' - \vec{a}^*\| \\
 &= \|\vec{a}^* - \vec{a} + [\hat{H}_F(\vec{a})]^{-1} \vec{g}_F(\vec{a})\| \\
 &= \|\vec{a}^* - \vec{a} + [H_F(\vec{a})]^{-1} \vec{g}_F(\vec{a}) + \vec{\Delta}_F(\vec{a})\| \\
 &= \|[H_F(\vec{a})]^{-1} \cdot [H_F(\vec{a})(\vec{a}^* - \vec{a}) + \vec{g}_F(\vec{a}) - \vec{g}_F(\vec{a}^*)] \\
 &\quad + \vec{\Delta}_F(\vec{a})\| \\
 &\leq \|[H_F(\vec{a})]^{-1}\| \cdot \|H_F(\vec{a})(\vec{a}^* - \vec{a}) + \vec{g}_F(\vec{a}) - \vec{g}_F(\vec{a}^*)\| \\
 &\quad + \|\vec{\Delta}_F(\vec{a})\| \\
 &\leq \frac{M}{2\mu} \|\vec{a} - \vec{a}^*\|^2 + \epsilon \\
 &= \frac{M}{2\mu} \delta^2 + \epsilon.
 \end{aligned} \tag{A19}$$

Here, we used $\vec{g}_F(\vec{a}^*) = \vec{0}$ to transform the third line to the fourth line, and (55), (57), and (59) to transform the fifth line to the sixth line. Using simple algebra, we can check that

$$\delta_- < \delta < \delta_+ \Rightarrow \frac{M}{2\mu} \delta^2 + \epsilon < \delta, \tag{A20}$$

and

$$\delta \leq \delta_- \Rightarrow \frac{M}{2\mu} \delta^2 + \epsilon \leq \delta_-, \tag{A21}$$

which means that the later part of the statement holds.

3. Proof of Lemma 3

Proof. First, let us see that

$$\delta_{n+1} \leq 2\epsilon \quad \text{if } \delta_n \leq 2\epsilon \tag{A22}$$

for a non-negative integer n . This immediately follows Lemma 2. According to it, $\delta_{n+1} < \delta_n$ if $\delta_- < \delta_n \leq 2\epsilon$, and $\delta_{n+1} \leq \delta_-$ if $\delta_n \leq \delta_-$ [note that $\delta_- < 2\epsilon < \delta_+$ holds under (61)]. Combining these, we obtain (A22).

Then, let us consider the following three cases of the initial deviation.

(i) $\delta_0 \leq 2\epsilon$.

From (A22), we immediately see that $\delta_n \leq 2\epsilon$ also for $n = 1, 2, \dots$.

(ii) $2\epsilon < \delta_0 \leq \sqrt{2\mu\epsilon/M}$.

In this case, according to Lemma 2, $\delta_1 \leq \frac{M}{2\mu}(\delta_0)^2 + \epsilon \leq 2\epsilon$. Therefore, by (A22), $\delta_n \leq 2\epsilon$ holds for $n = 1, 2, \dots$.

(iii) $\sqrt{2\mu\epsilon/M} < \delta_0 < \frac{\mu}{M}$.

We define

$$\tilde{n} := \left\lceil \log_2 \left(\frac{\ln \left(\frac{2M\epsilon}{\mu} \right)}{2 \ln \left(\frac{M\delta_0}{\mu} \right)} \right) \right\rceil,$$

which is positive in this case. In the sequence of the updates from $\vec{a}_0$ to $\vec{a}_{\tilde{n}}$, if $\delta_{n'} \leq \sqrt{2\mu\epsilon/M}$ for some $n' \in \{0, 1, \dots, \tilde{n} - 1\}$, $\delta_n \leq 2\epsilon$ holds for $n > n'$, as we discussed in case (ii). Otherwise, $\delta_n > \sqrt{2\mu\epsilon/M}$, and therefore $\delta_{n+1} \leq \frac{M}{2\mu}(\delta_n)^2 + \epsilon \leq$

$\frac{M}{\mu}(\delta_n)^2$ holds for $n = 0, 1, \dots, \tilde{n} - 1$, which means that

$$\delta_n \leq \frac{\mu}{M} \left(\frac{M\delta_0}{\mu} \right)^{2^n} \tag{A23}$$

for $n = 1, \dots, \tilde{n}$ and especially $\delta_{\tilde{n}} \leq \sqrt{2\mu\epsilon/M}$. Therefore, we see that $\delta_n \leq 2\epsilon$ for $n \geq \tilde{n} + 1$, as we discussed in case (ii).

In summary, the statement of the lemma has been proven in all cases.

4. Proof of Lemma 4

Proof. We let $\delta H_F(\vec{a})$ and $\delta \vec{g}_F(\vec{a})$ be the deviations of the estimated Hessian and gradient from the true values, that is,

$$\hat{H}_F(\vec{a}) =: H_F(\vec{a}) + \delta H_F(\vec{a}), \quad \vec{\hat{g}}_F(\vec{a}) =: \vec{g}_F(\vec{a}) + \delta \vec{g}_F(\vec{a}), \tag{A24}$$

respectively. Besides, we let $\delta H_{F,ij}(\vec{a})$ be the (i, j) th component of $\delta H_F(\vec{a})$ and $\delta g_{F,i}(\vec{a})$ be the i th component of $\delta \vec{g}_F(\vec{a})$. Furthermore, following the statement of the lemma, we assume that $\delta H_{F,ij}(\vec{a})$ and $\delta g_{F,i}(\vec{a})$ are bounded as follows:

$$|\delta H_{F,ij}(\vec{a})| \leq \epsilon'_H, \quad |\delta g_{F,i}(\vec{a})| \leq \epsilon'_g. \tag{A25}$$

First, we show that, under (68), or more loosely

$$\epsilon'_H < \frac{\mu}{d}, \tag{A26}$$

$\hat{H}_F(\vec{a})$ is positive-definite and therefore the update (52) from $\vec{a}$ is well-defined. Here, note that $\epsilon/4\delta_- \leq \epsilon/4\delta_- < 1/4$ since $\epsilon < \delta_-$, which can be shown by simple algebra under (61). From (A26), we obtain

$$\|\delta H_F(\vec{a})\| \leq \|\delta H_F(\vec{a})\|_F < \mu. \tag{A27}$$

On the other hand, as (A2), we can see that

$$|\hat{\lambda}_d - \lambda_d| \leq \|\delta H_F(\vec{a})\|, \tag{A28}$$

where λ_d and $\hat{\lambda}_d$ are the minimum eigenvalues of $H_F(\vec{a})$ and $\hat{H}_F(\vec{a})$, respectively. Combining (A27), (A28), and $\lambda_d > \mu$, we see

$$\hat{\lambda}_d \geq \lambda_d - \|\delta H_F(\vec{a})\| > 0, \tag{A29}$$

which means that $\hat{H}_F(\vec{a})$ is positive-definite.

When $\hat{H}_F(\vec{a})$ is invertible, considering up to the first-order perturbation with respect to ϵ'_H and ϵ'_g , we obtain

$$\begin{aligned}
 \vec{\Delta}_F(\vec{a}) &\approx -[H_F(\vec{a})]^{-1} \delta H_F(\vec{a}) [H_F(\vec{a})]^{-1} \vec{g}_F(\vec{a}) \\
 &\quad + [H_F(\vec{a})]^{-1} \delta \vec{g}_F(\vec{a}).
 \end{aligned} \tag{A30}$$

Using the following inequalities:

$$\|\delta H_F(\vec{a})\| \leq \|\delta H_F(\vec{a})\|_F \leq d\epsilon'_H, \tag{A31}$$

$$\|\delta \vec{g}_F(\vec{a})\| \leq d^{1/2} \epsilon'_g, \tag{A32}$$

and (55), we can evaluate (A30) as

$$\begin{aligned}
 \|\vec{\Delta}_F(\vec{a})\| &\leq \|[H_F(\vec{a})]^{-1}\| \cdot \|\delta H_F(\vec{a})\| \cdot \|[H_F(\vec{a})]^{-1}\| \|\vec{g}_F(\vec{a})\| \\
 &\quad + \|[H_F(\vec{a})]^{-1}\| \cdot \|\delta \vec{g}_F(\vec{a})\| \\
 &\leq \frac{d\epsilon'_H}{\mu} \|[H_F(\vec{a})]^{-1}\| \|\vec{g}_F(\vec{a})\| + \frac{d^{1/2} \epsilon'_g}{\mu}.
 \end{aligned} \tag{A33}$$

⁷Note that (61) means $\sqrt{\frac{2\mu\epsilon}{M}} > 2\epsilon$.

Since

$$\|[H_F(\vec{a})]^{-1}\vec{g}_F(\vec{a})\| \leq 2\delta \quad (\text{A34})$$

as shown later, we obtain $\|\vec{\Delta}_F(\vec{a}_n)\| \leq \epsilon$ from (A33) for ϵ'_H and ϵ'_g satisfying (68) and (67), respectively.

The remaining task is to show (A34). Note that $[H_F(\vec{a})]^{-1}\vec{g}_F(\vec{a})$ is the update difference from $\vec{a}$ with the errorless update (44). In light of this, let us define $\vec{a}'_{\text{NoErr}}$ as the result of the update (44) from $\vec{a}$ and $\delta'_{\text{NoErr}} := \|\vec{a}'_{\text{NoErr}} - \vec{a}^*\|$. Since $\delta < 2\mu/M$, $\delta'_{\text{NoErr}} \leq \delta$ holds by Lemma 2 [Eq. (62)] with $\epsilon = 0$. Therefore,

$$\begin{aligned} \|[H_F(\vec{a})]^{-1}\vec{g}_F(\vec{a})\| &= \|\vec{a}'_{\text{NoErr}} - \vec{a}\| \\ &\leq \|\vec{a}'_{\text{NoErr}} - \vec{a}^*\| + \|\vec{a} - \vec{a}^*\| \end{aligned}$$

$$\begin{aligned} &= \delta'_{\text{NoErr}} + \delta \\ &\leq 2\delta. \end{aligned} \quad (\text{A35})$$

5. Proof of Lemma 5

Proof. Assume that $\delta_n = \|\vec{a}_n - \vec{a}^*\| \leq \tilde{\delta}_0$. Then, $\epsilon'_H \leq \mu\epsilon/4\delta_n d$ because of (70). This means that the conditions on estimation errors (67) and (68) in Lemma 4 are satisfied for the update from $\vec{a}_n$. Since $\delta_n < \delta_+ \leq 2\mu/M$ is also satisfied, (69) holds by Lemma 4. Then, we see that $\delta_{n+1} \leq \max\{\delta_n, \delta_-\}$ is satisfied by Lemma 2, which means $\delta_{n+1} \leq \tilde{\delta}_0$. Using induction, we see that (69) holds for any n .

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