Quantum support vector machine for big feature and big data classification

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Supervised machine learning is the classification of new data based on already classified training examples. In this work, we show that the support vector machine, an optimized linear and non-linear binary classifier, can be implemented on a quantum computer, with exponential speedups in the size of the vectors and the number of training examples. At the core of the algorithm is a non-sparse matrix simulation technique to efficiently perform a principal component analysis and matrix inversion of the training data kernel matrix. We thus provide an example of a quantum big feature and big data algorithm and pave the way for future developments at the intersection of quantum computing and machine learning.

Machine learning can be separated into two branches, supervised and unsupervised learning [1-4]. In unsupervised learning, the task is to find structure in unlabeled data, such as clusters in a set of data points. Supervised learning involves a training set of already classified data, from which inferences are made to classify new data. In both cases, recent applications exhibit a growing number of features and input data. A support vector machine (SVM) is a supervised machine learning algorithm that classifies vectors in a feature space into one of two sets, given training data from the sets [5]. The machine operates by constructing the optimal hyperplane dividing the two sets, either in the original feature space or a higher-dimensional kernel space. The SVM can be formulated as a quadratic programming problem [6], which can be solved in time proportional to O(polyNM), with N the dimension of the feature space and M the number of training vectors. Ref. [7] introduced a least-squares version of the SVM and [8] describes a large-scale version of it. Binary classification was discussed in terms of Grover search in [9] and in the context of the adiabatic algorithm in [10–13].

In this paper, we show that a quantum support vector machine can achieve $O(\log NM)$ performance in both training and classification stages. The exponential speedup in N arises due to a fast quantum evaluation of inner products, discussed in a general machine learning context by us in [14]. For the exponential speedup in M, we re-express the SVM as an approximate least-squares problem [7] that allows for a quantum solution with the matrix inversion algorithm [15, 16]. To this end, we employ a recently-developed technique for the efficient simulation of non-sparse positive semi-definite matrices [17]. This enables a quantum parallel principal component analysis of the training data kernel and covariance matrices arising in this context and other machine learning algorithms [18–20]. We note another timely benefit of quantum machine learning: data privacy [14]. The user of the support vector machine operates with the training data as quantum states and can only sample from those states. The algorithm never requires the explicit O(MN) representation of all the features of each of the training examples, but generates the necessary data structure, the kernel matrix of inner products, in quantum parallel. Once the kernel matrix is generated, the individual features of the training data are fully hidden from the user.

Support vector machine. - Support vector machines represent a powerful method for performing linear and non-linear classification [5]. The task is to classify a vector into one of two classes, given M training data points of the form $\{(\vec{x}_j,y_j):\vec{x}_j\in\mathbb{R}^N,y_j=\pm 1\}_{j=1...M}, \text{ where }y_j=1 \text{ or }-1 \text{ depending on the class to which }\vec{x}_j \text{ belongs. In lin-}$ ear support vector machines, the method of classification is to find the maximum-margin hyperplane that divides the points with $y_i = 1$ from those with $y_i = -1$. The machine finds two parallel hyperplanes with normal vector \vec{u} , separated by the maximum possible distance $2/|\vec{u}|$, that separate the two classes of training data, and that have no data points in the margin between them. These hyperplanes are constructed so that $\vec{u} \cdot \vec{x}_j + b \ge 1$ for \vec{x}_j in the +1 class and that $\vec{u} \cdot \vec{x}_i + b \leq -1$ for \vec{x}_i in the -1 class, where b is proportional to the offset of the hyperplane. Thus, finding the maximum margin hyperplane consists of minimizing $|\vec{u}|^2/2$ subject to the inequality constraints $y_i(\vec{u} \cdot \vec{x}_i + b) \ge 1$ for all j. This is the primal formulation of the problem. To obtain the dual formulation, the Karush-Kuhn-Tucker multipliers α'_i are employed for the inequality constraints to first arrive at a min/max problem, which, defining $\alpha_i = y_i \alpha_i$, is formally solved by $\vec{u} = \sum_{j=1}^{M} \alpha_j \vec{x}_j$ and $b = y_j - \vec{u} \cdot \vec{x}_j$ (for those jwhere $\alpha_j \neq 0$), where $y_j \alpha_j \geq 0$ and $\sum_{j=1}^{M} \alpha_j = 0$. Only a few of the α_i are non-zero: these are the ones corresponding to the \vec{x}_i that lie on the two hyperplanes – the support vectors. Employing this solution for \vec{u} and b, the dual formulation is maximizing over $\vec{\alpha} = (\alpha_1, \dots, \alpha_M)^T$ the function:

$$L(\vec{\alpha}) = \sum_{j=1}^{M} y_j \alpha_j - \frac{1}{2} \sum_{j,k=1}^{M} \alpha_j K_{jk} \alpha_k, \tag{1}$$

subject to the constraints $\sum_{j=1}^{M} \alpha_j = 0$, $y_j\alpha_j \geq 0$. We have introduced the kernel matrix, a central quantity for supervised machine learning problems [18, 20], $K_{jk} = k(\vec{x}_j, \vec{x}_k) = \vec{x}_j \cdot \vec{x}_k$, defining the kernel function k(x,x'). More complicated non-linear kernels and soft margins will be studied below. Solving the dual form involves evaluating the M(M-1)/2 dot products $\vec{x}_j \cdot \vec{x}_k$ in the kernel matrix, and then finding the optimal α_j values by quadratic programming, which takes $O(M^3)$ in the non-sparse case [21]. As each dot

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product takes time O(N) to evaluate, the classical support vector algorithm takes time at least $O(M^2(N+M))$. The result is a binary classifier:

$$y(\vec{x}) = \operatorname{sign}\left(\sum_{j=1}^{M} \alpha_j k(\vec{x}_j, \vec{x}) + b\right). \tag{2}$$

Classification is O(MN), or O(N) for the linear kernel when

the vector $\sum_{j=1}^{M} \alpha_j \vec{x}_j$ is computed once. Quantum inner-product evaluation. — In the quantum setting, assume that we are given oracles for the training data that return quantum vectors $|\vec{x}_j\rangle = 1/|\vec{x}_j|\sum_{k=1}^N (\vec{x}_j)_k |k\rangle$, the norms $|\vec{x}_j|$, and the labels y_j , see the discussion in [14]. To evaluate a single dot product $\vec{x}_i \cdot \vec{x}_k = |\vec{x}_i| |\vec{x}_k| \langle \vec{x}_i | \vec{x}_k \rangle$, proceed as described in Ref. [14] to obtain $O(\log N/\epsilon)$ run time, where ϵ is the accuracy. Once all the dot products in the kernel matrix have been evaluated to accuracy ϵ , the optimal α_i can be identified by quadratic programming to the same degree of accuracy. To classify a vector \vec{x} to the +1 or -1 set in the quantum algorithm, assume that we are given \vec{x} as a normalized quantum vector $|x\rangle$ together with the normalization $|\vec{x}|$. We construct $|\vec{u}\rangle \propto \sum_{j=1}^{M} \alpha_j |\vec{x}_j\rangle$. Evaluate the dot product $\vec{u} \cdot \vec{x}$ as above and compare the result to $b = y_j - \vec{u} \cdot \vec{x}_j$. Comparing this quantum support vector machine with the classical support vector machine, we see that the run time of the quantum algorithm is $O(M^2(M + \log N/\epsilon))$, while the classical algorithm can scale as $O(M^2(M + \text{poly}(N)/\epsilon^2))$, depending on the distribution of the components of the \vec{x}_i . We now move on to the big data exponential speedup in M.

Preparation and simulation of the kernel matrix K/trK.-The kernel matrix plays a crucial role in the dual formulation Eq. (1) and the least-squares reformulation discussed in the next section. At this point we can already discuss efficient preparation and simulation methods for the normalized kernel matrix $\hat{K} = K/\text{tr}K$. Classically, setting up the kernel matrix takes $O(M^2N)$ run time. For the quantum mechanical preparation, first call the training data oracle with the state $1/\sqrt{M}\sum_{i=1}^{M}|i\rangle$. This prepares in quantum parallel the state $|\chi\rangle = 1/\sqrt{N_\chi} \sum_{i=1}^M |\vec{x}_i| |i\rangle |\vec{x}_i\rangle$, with $N_\chi = \sum_{i=1}^M |\vec{x}_i|^2$, in $O(\log NM)$ run time [22]. If we discard the training set register, we obtain the desired kernel matrix as a quantum density matrix. This can be seen from the partial trace ${\rm tr}_2\{|\chi\rangle\langle\chi|\}=\frac{1}{N_\chi}\sum_{i,j=1}^M\langle\vec{x}_j|\vec{x}_i\rangle|\vec{x}_i||\vec{x}_j||i\rangle\langle j|=\frac{K}{{\rm tr}K}.$ We will show how to use this state in a fully quantum mechanical algorithm to approximately solve the SVM. See the appendix for an independent estimation of the trace of K.

For quantum mechanically computing a matrix inverse such as \hat{K}^{-1} one needs to be able to efficiently simulate $e^{-i\hat{K}\Delta t}$. However, the kernel matrix \hat{K} is not sparse for the straightforward application of sparse simulation techniques [23, 24]. For the simulation of non-sparse symmetric or Hermitian matrices a strategy was developed in [17]. We adapt it to the present problem. Adopting a density matrix description to extend the space of possible transformations gives, for some quantum state ρ , $e^{-i\hat{K}\Delta t}$ ρ $e^{i\hat{K}\Delta t} = e^{-i\mathcal{L}_{\hat{K}}\Delta t}(\rho)$, where the superoperator notation $\mathcal{L}_K(\rho) = [K, \rho]$, or simply $\mathcal{L}_K = [K, \cdot]$, was defined. Applying the algorithm of [17] obtains:

$$e^{-i\mathcal{L}_{\hat{K}}\Delta t} \approx \operatorname{tr}_{1}\left\{e^{-iS\Delta t}\hat{K}\otimes(\cdot)e^{iS\Delta t}\right\}$$

$$= \mathbb{1} - i\Delta t[\hat{K},\cdot] + O(\Delta t^{2}).$$
(3)

Here, $S=\sum_{m,n=1}^M |m\rangle\langle n|\otimes |n\rangle\langle m|$ is the swap matrix of dimension $M^2\times M^2$. Eq. (3) is the operation that is implemented on the quantum computer performing the machine learning. For the time slice Δt , it consists of the preparation of an environment state K (see above) and the application of the global swap operator to the combined system/environment state followed by discarding the environmental degrees of freedom. This shows that the simulation of $e^{-i\hat{K}\Delta t}$ is possible with error $O(\Delta t^2)$. The efficient preparation and simulation of the training data kernel matrix, which appears in many machine learning problems [18, 20], potentially enables a wide range of supervised quantum machine learning algorithms.

Quantum least-squares support vector machine.— A key idea of this work is to employ the least-squares reformulation of the support vector machine developed in [7] that circumvents the quadratic programming and obtains the parameters from the solution of a linear equation system. The central simplification is to introduce slack variables e_i and replace the inequality constraints with equality constraints (using $y_i^2 = 1$):

$$y_i(\vec{u} \cdot \vec{x}_i + b) \ge 1 \to (\vec{u} \cdot \vec{x}_i + b) = y_i - y_i e_i. \tag{4}$$

In addition to the constraints, the implied Lagrange function contains a penalty term $\gamma/2\sum_{j=1}^M e_j^2$, where user-specified γ determines the relative weight of training error and SVM objective. Taking partial derivatives of the Lagrange function and eliminating the variables \vec{u} and e_i leads to a least-squares approximation of the problem:

$$F\begin{pmatrix} b \\ \vec{\alpha} \end{pmatrix} \equiv \begin{pmatrix} 0 & \vec{1}^T \\ \vec{1} & K + \gamma^{-1} \mathbb{1} \end{pmatrix} \begin{pmatrix} b \\ \vec{\alpha} \end{pmatrix} = \begin{pmatrix} 0 \\ \vec{y} \end{pmatrix}. \quad (5)$$

Here, $K_{ij} = \vec{x}_i^T \cdot \vec{x}_j$ is again the symmetric kernel matrix, $\vec{y} = (y_1, \cdots, y_M)^T$, and $\vec{1} = (1, \cdots, 1)^T$. The matrix F is $(M+1) \times (M+1)$ dimensional. The additional row and column with the $\vec{1}$ arise because of a non-zero offset b. The α_i take on the role as distances from the optimal margin. The support vector machine parameters are determined schematically by $(b, \vec{\alpha}^T)^T = F^{-1}(0, \vec{y}^T)^T$. As with the quadratic programming formulation, the complexity of the least-squares support vector machine is $O(M^3)$ [21].

For the quantum support vector machine, we would like to generate a quantum state $|b, \vec{\alpha}\rangle$ describing the hyperplane with the matrix inversion algorithm [15] and then classify a state $|x\rangle$. For application of the quantum matrix inversion algorithm one needs to be able to efficiently simulate the matrix exponential of F. First, the matrix F is divided as: $F = J + K_{\gamma}$, with $J = \begin{pmatrix} 0 & \vec{1}^T \\ \vec{1} & 0 \end{pmatrix}$ and $K_{\gamma} = \begin{pmatrix} 0 & 0 \\ 0 & K + \gamma^{-1} \mathbb{1} \end{pmatrix}$. The matrix J is efficiently quantum mechanically simula-

ble [23] ("star" graph). The two nonzero eigenvalues of J

are $\lambda_{\pm}^{\rm star}=\pm\sqrt{M}$ and the corresponding eigenstates are $|\lambda_{\pm}^{\rm star}\rangle=\frac{1}{\sqrt{2}}\left(|0\rangle\pm\frac{1}{\sqrt{M}}\sum_{k=1}^{M}|k\rangle\right)$. The identity matrix $\gamma^{-1}\mathbbm{1}$ is trivially simulable. For the simulation of $K/{\rm tr}K$, proceed according Eq. (3). Define $\hat{F}=F/{\rm tr}F=J/{\rm tr}K_{\gamma}+\hat{K}_{\gamma}$, with $\hat{K}_{\gamma}=K_{\gamma}/{\rm tr}K_{\gamma}$. The Lie product formula gives $e^{-i\hat{F}\Delta t}=e^{-iJ\Delta t/{\rm tr}K_{\gamma}}e^{-i1\Delta t/{\rm tr}K_{\gamma}}e^{-iK\Delta t/{\rm tr}K_{\gamma}}+O(\Delta t^2)=e^{-iJ\Delta t'/{\rm tr}K}e^{-i1\Delta t'/{\rm tr}K}e^{-i\hat{K}\Delta t'}+O(\Delta t^2)$, with $\Delta t'=\frac{{\rm tr}K}{{\rm tr}K_{\gamma}}\Delta t$. See the appendix for the evaluation of ${\rm tr}K$. This $e^{-i\hat{F}\Delta t}$ is employed conditionally in phase estimation.

We assume that the normalized quantum state corresponding to the right-hand side of Eq. (5), $|\tilde{y}\rangle=1/\sqrt{M}\sum_{k=1}^M y_k|k\rangle$, can be efficiently prepared. We can formally expand this state into eigenstates $|u_j\rangle$ of \hat{F} with corresponding eigenvalues λ_j , $|\tilde{y}\rangle=\sum_{j=1}^{M+1}\langle u_j|\tilde{y}\rangle|u_j\rangle$. With a register for storing an approximation of the eigenvalues (initialized to $|0\rangle$), phase estimation generates a state which is close to the ideal state storing the respective eigenvalue:

$$|\tilde{y}\rangle|0\rangle \to \sum_{j=1}^{M+1} \langle u_j|\tilde{y}\rangle|u_j\rangle|\lambda_j\rangle \to \sum_{j=1}^{M+1} \frac{\langle u_j|\tilde{y}\rangle}{\lambda_j}|u_j\rangle.$$
 (6)

The second step inverts the eigenvalue and is obtained as in [15] by performing a controlled rotation and uncomputing the eigenvalue register. In the basis of training set labels, the expansion coefficients of the new state are the desired support vector machine parameters:

$$|b, \vec{\alpha}\rangle = \frac{1}{\sqrt{C}} \left(b|0\rangle + \sum_{k=1}^{M} \alpha_k |k\rangle \right),$$
 (7)

where $C = b^2 + \sum_{k=1}^{M} \alpha_k^2$.

Classification.— We have now trained the quantum SVM and would like to classify a query state $|x\rangle$. From the state $|b, \vec{\alpha}\rangle$ in Eq. (7), construct by calling the training-data oracle:

$$|\tilde{u}\rangle = \frac{1}{\sqrt{N_{\tilde{u}}}} \left(b|0\rangle|0\rangle + \sum_{k=1}^{M} \alpha_k |\vec{x}_k||k\rangle|\vec{x}_k\rangle \right),$$
 (8)

with $N_{\tilde{u}}=b^2+\sum_{k=1}^M\alpha_k^2|\vec{x}_k|^2.$ In addition, construct the query state:

$$|\tilde{x}\rangle = \frac{1}{\sqrt{N_{\tilde{x}}}} \left(|0\rangle|0\rangle + \sum_{k=1}^{M} |\vec{x}||k\rangle|\vec{x}\rangle \right).$$
 (9)

with $N_{\tilde{x}}=M|\vec{x}|^2+1$. For the classification, we perform a swap test. Using an ancilla, construct the state $|\psi\rangle=\frac{1}{\sqrt{2}}(|0\rangle|\tilde{u}\rangle+|1\rangle|\tilde{x}\rangle)$ and measure the ancilla in the state $|\phi\rangle=\frac{1}{\sqrt{2}}(|0\rangle-|1\rangle)$. The measurement has the success probability $P=|\langle\psi|\phi\rangle|^2=\frac{1}{2}(1-\langle\tilde{u}|\tilde{x}\rangle)$. The inner product is given by $\langle\tilde{u}|\tilde{x}\rangle=\frac{1}{\sqrt{N_{\tilde{x}}N_{\tilde{u}}}}\left(b+\sum_{k=1}^{M}\alpha_k|\vec{x}_k||\vec{x}|\langle\vec{x}_k|\vec{x}\rangle\right)$. If P<1/2 we classify $|x\rangle$ as +1, otherwise -1.

Kernel matrix compression and error analysis. – In this section, we show that quantum matrix inversion essentially performs a kernel matrix principal component analysis and give a run time/error analysis of the quantum algorithm. The matrix under consideration, $\hat{F} = F/\text{tr}F$, contains the kernel matrix $\hat{K}_{\gamma} = K_{\gamma}/\mathrm{tr}K_{\gamma}$ and an additional row and column due to the offset parameter b. In case the offset is negligible, the problem reduces to matrix inversion of the kernel matrix \hat{K}_{γ} only. For any finite $\gamma, \hat{K}_{\gamma} > 0$, which means that \hat{K}_{γ} is invertible. The condition number κ of \hat{F} plays an important role in the classical and quantum matrix inversion. The positive eigenvalues of \hat{F} are dominated by the eigenvalues of \hat{K}_{γ} . In addition, \hat{F} has one additional negative eigenvalue which is involved in determining the offset parameter b, see the appendix. The maximum eigenvalue of \hat{K}_{γ} is no greater than 1 and the minimum eigenvalue is O(1/M). The minimum eigenvalue can be seen by the possibility of having a training example that has (almost) zero overlap with the other training examples. Because of the normalization the eigenvalue will be O(1/M) and the condition number is potentially O(M) in this case. Such a condition number would prevent the exponential quantum speedup in M [15]. To remedy this, we define a constant ϵ_K such that only the eigenvalues in the interval $\epsilon_K \leq |\lambda_i| \leq 1$ are taken into account, essentially defining an effective condition number $\kappa_{\rm eff} = 1/\epsilon_K$. Then, the filtering procedure described in [15] is employed in the phase estimation using this $\kappa_{\rm eff}$. A three dimensional auxiliary register is attached to the quantum state and, when multiplying the inverse $1/\lambda_i$ for each eigenstate as in Eq. (6), appropriately defined filtering functions discard eigenvalues below ϵ_K . The desired outcome is obtained by post-selecting the auxiliary register.

The legitimacy of this kernel matrix compression can be rationalized by its equivalence to principal component analysis. Define the $N \times M$ data matrix $X = (\vec{x}_1, \dots, \vec{x}_M)$. The $M \times M$ kernel matrix is given by $K = X^T X$. The $N \times N$ covariance matrix is given by $\Sigma = XX^T = \sum_{m=1}^M \vec{x}_m \vec{x}_m^T$. If the data is assumed to be standardized, principal component analysis [4] keeps the directions in the data that have the largest variance, which is equivalent to keeping the eigenvectors of Σ with the largest eigenvalues. The matrices XX^T and X^TX have the same eigenvalues, except for zero eigenvalues. Thus, the principal component idea directly translates into the kernel space. Removing small eigenvalues of the kernel matrix removes small eigenvalues of the covariance matrix. Keeping the large eigenvalues of the kernel matrix retains the principal components of the covariance matrix. In the present quantum algorithm, the kernel matrix compression (and thus the principal component analysis) is performed in quantum parallel by phase estimation.

We continue with a discussion of the run time of the quantum algorithm [15]. The interval Δt can be written as $\Delta t = t_0/T$ where T is the number of time steps in the phase estimation and the total evolution time t_0 determines the error of the phase estimation. The swap matrix used in Eq. (3) is 1-sparse and $e^{-iS\Delta t}$ for is efficiently simulable in negligible time

 $\tilde{O}(\log(M)\Delta t)$ [24]. The \tilde{O} notation suppresses more slowly growing factors, such as a $\log^* M$ factor [15, 24]. For the phase estimation, the propagator $e^{-i\mathcal{L}_{\hat{F}}\Delta t}$ is simulated with error $O(\Delta t^2 ||\hat{F}||^2)$, see Eq (3). With the spectral norm for a matrix A, $||A|| = \max_{|\vec{v}|=1} |A\vec{v}|$, we have $||\hat{F}|| = O(1)$. Taking powers of this propagator, $e^{-i\mathcal{L}_F\tau\Delta t}$ for $\tau=0,\cdots,T-1$, leads to an error of maximally $\epsilon = O(T\Delta t^2) = O(t_0^2/T)$. Thus, the run time is $T=O(t_0^2/\epsilon)$. Taking into account the preparation of the kernel matrix in $O(\log MN)$, the run time is thus $O(t_0^2 \log MN/\epsilon)$. The relative error of λ^{-1} by phase estimation is given by $O(1/t_0\lambda) \leq O(1/t_0\epsilon_K)$ for $\lambda \geq \epsilon_K$. If t_0 is taken $O(\kappa_{\text{eff}}/\epsilon) = O(1/\epsilon_K \epsilon)$ this error is $O(\epsilon)$. The run time is thus $\tilde{O}(\log MN/\epsilon_K^2\epsilon^3)$. Repeating the algorithm for $O(\kappa_{\rm eff})$ times to achieve a constant success probability of the post-selection step obtains a final run time of $O(\kappa_{\text{eff}}^3 \log MN/\epsilon^3)$. To summarize, we find a quantum support vector machine that scales as $O(\log MN)$, which implies a quantum advantage in situations where many training examples are involved ("quantum big data").

Nonlinear support vector machines.— One of the most powerful uses of support vector machines is to perform nonlinear classification [5]. Perform a nonlinear mapping $\vec{\phi}(\vec{x}_j)$ into a higher-dimensional vector space. Thus, the kernel function becomes a nonlinear function in \vec{x} :

$$k(\vec{x}_i, \vec{x}_k) = \vec{\phi}(\vec{x}_i) \cdot \vec{\phi}(\vec{x}_k). \tag{10}$$

For example, $k(\vec{x}_j, \vec{x}_k) = (\vec{x}_j \cdot \vec{x}_k)^d$. Now perform the SVM classification in the higher-dimensional space. The separating hyperplanes in the higher-dimensional space now correspond to separating nonlinear surfaces in the original space.

The ability of quantum computers to manipulate high-dimensional vectors affords a natural quantum algorithm for polynomial kernel machines. Simply map each vector $|\vec{x}_j\rangle$ into the d-times tensor product $|\phi(\vec{x}_j)\rangle \equiv |\vec{x}_j\rangle \otimes \ldots \otimes |\vec{x}_j\rangle$ and use the feature that $\langle \phi(\vec{x}_j)|\phi(\vec{x}_k)\rangle = \langle \vec{x}_j|\vec{x}_k\rangle^d$. Arbitrary polynomial kernels can be constructed using this trick. The optimization using a nonlinear, polynomial kernel in the original space now becomes a linear hyperplane optimization in the d-times tensor product space. Considering only the speedup in the vector space dimension, the nonlinear d-level polynomial quantum kernel algorithm to accuracy ϵ then runs in time $O(d \log N/\epsilon)$. Note that, in contrast to classical kernel machines, the exponential quantum advantage in evaluating inner products allows quantum kernel machines to perform the kernel evaluation directly in the higher dimensional space.

Conclusion.— In this work, we have shown that an important classifier in machine learning, the support vector machine, can be implemented quantum mechanically. We have obtained exponential speedups in feature size and the number of training data, thus providing one example of a quantum "big data" speedup. We have considered a least-squares formulation of the support vector machine, which allows the use of phase estimation and the quantum matrix inversion algorithm. To this end, we have employed a newly-developed non-sparse simulation technique for Hermitian positive semi-definite matrices. The speed of the quantum algorithm is max-

imized when the training data kernel matrix is dominated by a relatively small number of principal components. In summary, with the quantum support vector machine we have shown an efficient quantum implementation of an important machine learning algorithm, which also provides advantages in terms of data privacy and could be used as a component in a larger quantum neural network.

This work was supported by DARPA, NSF, ENI, Google, and Jeffrey Epstein.

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APPENDIX: THE OFFSET PARAMETER b

The matrix \hat{F} is not positive definite (the determinant of the upper 2×2 minor is negative). The positive eigenvalues of \hat{F} are dominated by the positive eigenvalues of \hat{K}_{γ} . To get an idea of the single negative eigenvalue of \hat{F} , which is related the offset parameter b, note that the eigenvalues of only the matrix $J/{\rm tr}K_{\gamma}$ are $\lambda_{\pm}^{\rm star}/O(M)=O(1/\sqrt{M})$. Thus, the negative eigenvalue of \hat{F} is potentially too small to be resolved by the phase estimation and the offset parameter b cannot be determined. One way to handle this issue is to center the data. Compute the centroid of the training data similar to the quantum k-means algorithm shown in [14] (ignoring the labels y_j). The re-centered training vectors are then used for the preparation of the kernel matrix and subsequent matrix inversion.

However, there exist cases for which the negative eigenvalue is O(1) and can thus be resolved by choosing ϵ_K appropriately. To show this, use the property of the determinant for block matrices, for $\lambda < 1/(\gamma {\rm tr} K_\gamma)$, to obtain for the characteristic polynomial:

$$0 = \det(\hat{F} - \lambda \mathbb{1}_{M+1}) = \det(\hat{K}_{\gamma} - \lambda \mathbb{1}_{M}) f(\lambda), \quad (11)$$

with the Schur complement $f(\lambda) = -\lambda - \hat{1}^T (\hat{K}_\gamma - \lambda \mathbb{1}_M)^{-1} \hat{1}$, where $\hat{1} = \vec{1}/\text{tr}K_\gamma$. Since \hat{K}_γ does not have any eigenvalues $< 1/(\gamma \text{tr}K_\gamma)$, we investigate the relation $f(\lambda) = 0$ to obtain information about the single negative eigenvalue λ_- . Note that $f(-|\lambda|) = |\lambda| - \hat{1}^T (\hat{K}_\gamma + |\lambda| \mathbb{1}_M)^{-1} \hat{1}$, and $\hat{1}^T (\hat{K}_\gamma + |\lambda| \mathbb{1}_M)^{-1} \hat{1} > 0$ since $\hat{K}_\gamma + |\lambda| \mathbb{1}_M$ is positive

definite. Note also that with the eigendecomposition $\hat{K}_{\gamma} = \sum_{j=1}^{M} \hat{k}_{j} \vec{k}_{j} \vec{k}_{j}^{T}$, with the eigenvalues $1/(\gamma \mathrm{tr} K_{\gamma}) \leq \hat{k}_{j} \leq 1$ and the corresponding normalized eigenvectors \vec{k}_{j} , we have $(\hat{K}_{\gamma} + |\lambda| \mathbb{1}_{M})^{-1} = \sum_{j=1}^{M} \frac{1}{|\lambda| + \hat{k}_{j}} \vec{k}_{j} \vec{k}_{j}^{T}$. The problem becomes $0 = |\lambda| - \sum_{j=1}^{M} \frac{1}{|\lambda| + \hat{k}_{j}} \beta_{j}$, with $\beta_{j} = (\vec{k}_{j}^{T} \cdot \hat{1})^{2}$, which is equivalent to $1 = \sum_{j=1}^{M} \frac{1}{|\lambda|^{2} + |\lambda| \hat{k}_{j}} \beta_{j}$. The special case when $\beta_{j} = O(1/M)$ occurs if the sum of components of \vec{k}_{j} is $O(\sqrt{M})$, for all j. Thus, the remainder of the terms in the sum determining $|\lambda|$ is O(1), because M O(1/M) terms need to add up to 1. In this case, λ_{-} is O(1). Which avenue is to be taken, centering the data or choosing a feasible ϵ_{K} , can be determined by cross-validation [4]. That is, using part of the training set for training and another part for classification to determine the correctness of the resulting SVM classifier.

APPENDIX: ESTIMATING THE TRACE OF THE KERNEL MATRIX

The trace of the kernel matrix can be efficiently evaluated, similar to [14]. Generate the Hamiltonian $H_{\rm tr}=\sum_{j=1}^M|\vec{x}_j||j\rangle\langle j|\otimes\sigma_x$ from the quantum access to the norms due to the training-data oracle. Applying $e^{-iH_{\rm tr}t}$ to the state $|\psi\rangle=1/\sqrt{M}\sum_{j=1}^M|j\rangle|0\rangle$ results in $|\psi(t)\rangle=1/\sqrt{M}\sum_{j=1}^M(\cos(|\vec{x}_j|t)|j\rangle|0\rangle-i\sin(|\vec{x}_j|t)|j\rangle|1\rangle)$. Choose t such that $|\vec{x}_j|t\ll 1$, for all j, and measure the ancilla in the $|1\rangle$ state. This succeeds with probability $1/M\sum_{j=1}^M|\vec{x}_j|^2t^2$, which allows the estimation of the trace of K, $\sum_{j=1}^M|\vec{x}_j|^2$.