Title: Classification on a quantum computer: Linear regression and ensemble methods

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Abstract: Quantum machine learning algorithms usually translate a machine learning methods into an algorithm that can exploit the advantages of quantum information processing. One approach is to tackle methods that rely on matrix inversion with the quantum linear system of equations routine. We give such a quantum algorithm based on unregularised linear regression. Opposed to closely related work from Wiebe, Braun and Lloyd [PRL 109 (2012)] our scheme focuses on a classification task and uses a different combination of core routines that allows us to process non-sparse inputs, and significantly improves the dependence on the condition number. The second part of the talk presents an idea that transcends the reproduction of classical results. Instead of considering a single trained classifier, practicioners often use ensembles of models to make predictions more robust and accurate. Under certain conditions, having infinite ensembles can lead to good results. We introduce a quantum sampling scheme that uses the parallelism inherent to a quantum computer in order to sample from 'exponentially large' ensembles that are not explicitely trained.

Prediction on a quantum computer: Linear regression and ensemble methods.

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QML Conference 8-12 August 2016



### CONTENT

- 1. Introduction
- 2. Quantum Machine Learning
- 3. Linear Regression on a Quantum Computer
- 4. Conclusion



Given a data set of inputs and their respective target outputs, predict the output for a new input.



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#### Input

# last month's oil price search history of a user insurance customers text images

## Output tomorrow's oil price chance to click on a car ad chance of claiming links to terrorism? cat, dog or plane?



Given a data set  $\mathcal{D} = \{(x^{(1)}, y^{(1)}), ..., (x^{(M)}, y^{(M)})\}$  of inputs  $x^{(m)} \in \mathcal{X}$  and their respective target outputs  $y^{(m)} \in \mathcal{Y}$ , predict the output  $\tilde{y} \in \mathcal{Y}$  for a new input  $\tilde{x} \in \mathcal{X}$ .

#### Input

#### Output

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Given a data set  $\mathcal{D} = \{(x^{(1)}, y^{(1)}), ..., (x^{(M)}, y^{(M)})\}$  of inputs  $x^{(m)} \in \mathbb{R}^N$  and their respective target outputs  $y^{(m)} \in \mathbb{R}$ , predict the output  $\tilde{y} \in \mathbb{R}$  for a new input  $\tilde{x} \in \mathbb{R}^N$ .

#### Input

#### Output

last month's oil price search history of a user insurance customers text images tomorrow's oil price chance to click on a car ad chance of claiming links to terrorism? cat, dog or plane?



























Quantum approaches to machine learning:

 Universal quantum computer for matrix inversion problems (SVMs, PCA, LR)



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- Quantum annealer for optimisation problems (BMs)



QML

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Quantum approaches to machine learning:

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Quantum approaches to machine learning:

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- Quantum states as sampling distributions (BMs, EMs)
- Quantum states as probabilistic models (HMMs, BNs)
- Theory of quantum learning



# **GENERAL IDEA**

Doing linear algebra with amplitudes.

amplitude	probability	state
$a_0$	$ a_0 ^2$	$ 000\rangle$
$a_1$	$ a_1 ^2$	$ 001\rangle$
$a_2$	$ a_2 ^2$	$ 010\rangle$
:	:	÷
$a_7$	$ a_{7} ^{2}$	$ 111\rangle$



QUANTUM LINEAR REGRESSION

### **RELATED WORK**

PRL 109, 050505 (2012)

#### PHYSICAL REVIEW LETTERS

week ending 3 AUGUST 2012

#### G Quantum Algorithm for Data Fitting

Nathan Wiebe,<sup>1</sup> Daniel Braun,<sup>2,3</sup> and Seth Lloyd<sup>4</sup> <sup>1</sup>Institute for Quantum Computing and Department of Combinatorics and Optimization, University of Waterloo, 200 University Ave., West, Waterloo, Ontario, Canada <sup>2</sup>Laboratoire de Physique Théorique, Université Paul Sabatier, 118, Route de Narbonne, F-31062 Toulouse, France <sup>3</sup>CNRS, LPT (IRSAMC), F-31062 Toulouse, France

<sup>4</sup>Department of Mechanical Engineering, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA (Received 1 May 2012; published 2 August 2012)

We provide a new quantum algorithm that efficiently determines the quality of a least-squares fit over an exponentially large data set by building upon an algorithm for solving systems of linear equations efficiently [Harrow et al., Phys. Rev. Lett. 103, 150502 (2009)]. In many cases, our algorithm can also efficiently find a concise function that approximates the data to be fitted and bound the approximation error. In cases where the input data are pure quantum states, the algorithm can be used to provide an efficient parametric estimation of the quantum state and therefore can be applied as an alternative to full quantum-state tomography given a fault tolerant quantum computer.

DOI: 10.1103/PhysRevLett.109.050505

PACS numbers: 03.67.Ac, 02.60.Ed, 42.50.Dv

Invented as early as 1794 by Carl Friedrich Gauss, fitting data to theoretical models has become over the centuries one of the most important tools in all of quantitative science [1]. Typically, a theoretical model depends on a number of parameters, and leads to functional relations between data that will depend on those parameters. Fitting a large amount are beyond classical computability [8,9]. Recently, a quantum algorithm (called HHL in the following) was introduced that efficiently solves a linear equation,  $\mathbf{Fx} = \mathbf{b}$ , with given vector  $\mathbf{b}$  of dimension N and sparse Hermitian matrix  $\mathbf{F}$  [10], "Efficient solution" means that the expectation value  $\langle \mathbf{x} | \mathbf{M} | \mathbf{x} \rangle$  of an arbitrary poly-size Hermitian operator  $\mathbf{M}$  can



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#### QUANTUM LINEAR REGRESSION



Model:  
$$y = f(\mathbf{x}, \mathbf{w}) = \mathbf{x}^T \mathbf{\hat{w}}$$

#### QUANTUM LINEAR REGRESSION



## Ordinary Least Squares:

$$\hat{\mathbf{w}} = \min_{\mathbf{w}} ||\mathbf{X}\mathbf{w} - \mathbf{y}||^2$$

 $y^{(M)}$ 

 $\mathbf{X} = \begin{pmatrix} \dots \mathbf{x}^{(1)} \dots \end{pmatrix}$  $\vdots \\ \dots \mathbf{x}^{(M)} \dots \end{pmatrix}$ 

 $\mathbf{y} =$ 



#### QUANTUM LINEAR REGRESSION



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QUANTUM LINEAR REGRESSION

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$$\mathbf{\hat{w}} = \sum_{r=1}^{R} \sqrt{\lambda_r}^{-1} \mathbf{v}_r \mathbf{u}_r^T \mathbf{y}$$

 $\sqrt{\lambda_r}$  - rth singular value of X  $\mathbf{v}_r$  - rth right singular vector of X  $\mathbf{u}_r$  - rth left singular vector of X

Model:  
$$y = f(\mathbf{x}, \mathbf{w}) = \mathbf{x}^T \hat{\mathbf{w}}$$

QUANTUM LINEAR REGRESSION





 $\begin{aligned} \lambda_r &- r \text{th eigenvalue of } \mathbf{X}^T \mathbf{X}, \mathbf{X} \mathbf{X}^T \\ \mathbf{v}_r &- r \text{th eigenvector of } \mathbf{X}^T \mathbf{X} \\ \mathbf{u}_r &- r \text{th eigenvector of } \mathbf{X} \mathbf{X}^T \end{aligned}$ 

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QUANTUM LINEAR REGRESSION
#### **DESIRED SOLUTION**





 $\lambda_r$  - rth eigenvalue of  $\mathbf{X}^T \mathbf{X}, \mathbf{X} \mathbf{X}^T$  $\mathbf{v}_r$  - rth eigenvector of  $\mathbf{X}^T \mathbf{X}$  $\mathbf{u}_r$  - rth eigenvector of  $\mathbf{X} \mathbf{X}^T$ 

Model:  $y = f(\mathbf{x}, \mathbf{w}) = \mathbf{x}^T \mathbf{\hat{w}}$ 

#### QUANTUM LINEAR REGRESSION

#### CAN WE DO THIS ON A QCOMPUTER?

$$\tilde{y} = \sum_{r=1}^{R} \sqrt{\lambda_r^{-1}} \left( \tilde{\mathbf{x}}^T \mathbf{v}_r \right) \left( \mathbf{u}_r^T \mathbf{y} \right)$$

 $\rightarrow$  Idea:

$$\tilde{y} = \sum_{r=1}^{R} \sqrt{\lambda_r^{-1}} \langle \psi_{\tilde{\mathbf{x}}} | \psi_{\mathbf{v}_r} \rangle \langle \psi_{\mathbf{u}_r} | \psi_{\mathbf{y}} \rangle$$

We need a quantum algorithm that produces quantum state vectors corresponding to the desired eigenvectors and eigenvalues.



## AMPLITUDE ENCODING

Associate the amplitudes of quantum state vector with the entries of a classical vector  $\mathbf{a} \in \mathbb{R}^{2^n}$ :

$$\mathbf{a} = \begin{pmatrix} a_0 \\ \vdots \\ a_{2^n - 1} \end{pmatrix} \iff |\psi_{\mathbf{a}}\rangle = \sum_{j=0}^{2^n - 1} a_j |j\rangle$$

QUANTUM LINEAR REGRESSION

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Step 1: State preparation.

$$\begin{split} |\psi_{\mathbf{X}}\rangle &= \sum_{j=1}^{N} \sum_{m=1}^{M} x_{j}^{(m)} |j\rangle |m\rangle \\ |\psi_{\mathbf{y}}\rangle &= \sum_{\mu=1}^{M} y^{(\mu)} |\mu\rangle , \\ |\psi_{\tilde{\mathbf{x}}}\rangle &= \sum_{\gamma=1}^{N} \tilde{x}_{\gamma} |\gamma\rangle . \end{split}$$



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Step 1: State preparation.

The reduced density matrix of  $|\psi_{\mathbf{X}}\rangle$  is equivalent to  $\mathbf{X}^T\mathbf{X}$ :

$$\operatorname{tr}_{m}\{|\psi_{\mathbf{X}}\rangle\langle\psi_{\mathbf{X}}|\} = \rho_{\mathbf{X}^{\dagger}\mathbf{X}} = \sum_{j,j'=1}^{N} \sum_{m=1}^{M} x_{j}^{(m)} x_{j'}^{(m)*} |j\rangle\langle j'|$$

QUANTUM LINEAR REGRESSION

Step 2: Extracting the singular values.

Idea [Harrow, Hassidim, Lloyd (2009)]: Solve  $\mathbf{A}\mathbf{x} = \mathbf{b}$  on a quantum computer.

$$e^{-i\mathbf{A}\Delta t} |\psi_{\mathbf{b}}\rangle = e^{-i\mathbf{A}\Delta t} \sum_{j} \beta_{j} |\psi_{\mathbf{u}_{j}}\rangle = \sum_{j} \beta_{j} e^{-i\lambda_{j}\Delta t} |\psi_{\mathbf{u}_{j}}\rangle$$
$$QPE \rightarrow \sum_{j} \beta_{j} |\psi_{\mathbf{u}_{j}}\rangle |\lambda_{j}\rangle$$

QUANTUM LINEAR REGRESSION

Step 2: Extracting the singular values.

Idea [Lloyd, Mohseni, Rebentrost (2014)]: 'Exponentiate' density matrices.

$$e^{-i\rho\Delta t} |\psi_{\mathbf{b}}\rangle = e^{-i\rho\Delta t} \sum_{j} \beta_{j} |\psi_{\mathbf{u}_{j}}\rangle = \sum_{j} \beta_{j} e^{-i\lambda_{j}\Delta t} |\psi_{\mathbf{u}_{j}}\rangle$$
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QUANTUM LINEAR REGRESSION

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Step 2: Extracting the singular values.

Idea Quantum Linear Regression Algorithm:

$$e^{-i\rho_{\mathbf{X}^{\dagger}\mathbf{X}^{\Delta}t}}\left|\psi_{\mathbf{X}}\right\rangle = \sum_{r=1}^{R} \sqrt{\lambda_{r}} e^{-i\lambda_{j}\Delta t} \left|\psi_{\mathbf{v}_{r}}\right\rangle \left|\psi_{\mathbf{u}_{r}}\right\rangle$$

QPE 
$$\rightarrow \sum_{r=1}^{R} \sqrt{\lambda_r} |\psi_{\mathbf{v}_r}\rangle |\psi_{\mathbf{u}_r}\rangle |\lambda_r\rangle$$

QUANTUM LINEAR REGRESSION

Step 3: Inverting the singular values.

From [Harrow, Hassidim, Lloyd (2009)]:

 $\sum_{r=1}^{R} \sqrt{\lambda_r} |\psi_{\mathbf{v}_r}\rangle |\psi_{\mathbf{u}_r}\rangle |\lambda_r\rangle \left( \sqrt{1 - \left(\frac{c}{\lambda_r}\right)^2} |0\rangle + \frac{c}{\lambda_r} |1\rangle \right)$ 

$$\mathrm{CM} \to \frac{1}{\sqrt{p(1)}} \sum_{r=1}^{R} \frac{c}{\sqrt{\lambda_r}} |\psi_{\mathbf{v}_r}\rangle |\psi_{\mathbf{u}_r}\rangle$$

QUANTUM LINEAR REGRESSION

*Step 4: Classification of a new input.* Define

$$\begin{aligned} |\psi_1\rangle &:= \frac{1}{\sqrt{p(1)}} \sum_{r=1}^R \frac{c}{\sigma^r} |v^r\rangle |u^r\rangle \,, \\ |\psi_2\rangle &:= |\psi_{\mathbf{y}}\rangle |\psi_{\tilde{\mathbf{x}}}\rangle \,. \end{aligned}$$

Prepare

$$\frac{1}{\sqrt{2}}(\ket{\psi_1}\ket{0}+\ket{\psi_2}\ket{1}),$$

and the offdiagonal element of the ancilla's density matrix reads

$$\rho_{21} = \rho_{12} \propto \sum_r (\sqrt{\lambda_r^{-1}}) \sum_j v_j^r \tilde{x}_j \sum_m u_m^r y^{(m')}$$

QUANTUM LINEAR REGRESSION



#### SUMMARY

- Quantum algorithm for unregularised linear regression
- Works for low-rank approximable 'covariance matrices'
- Exponentially fast in the dimension and number of training data if state preparation for free















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