Quantum algorithms for linear regression

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Background

Quantum computing

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Solving these problems are based on quantum algorithms.

Quantum linear algebra

One plausible problem domain where quantum computers could be applied is linear algebra.

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[2] Harrow, Hassidim, Lloyd '08
[3] Gilyén et al '18
[4] Lloyd et al '20

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- Computing eigenvalues [1]
- Solving linear systems [2]
- Singular value decomposition [3]
- Polar decomposition [4]
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In this talk, I will mainly focus on the linear system problem.

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Quantum state: a basic object of quantum computing

Quantum state: $|\psi\rangle = \sum_{i=0}^{n-1} a_i |i\rangle$, where $\sum_i |a_i|^2 = 1$. Each $|i\rangle$ stands for a classical state, and $|\psi\rangle$ is a superposition of these states. Each state has a certain amplitude.

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- measure it: see $|i\rangle$ with probability $|a_i|^2 \to$ sampling. This is one way that we get useful information from $|\psi\rangle$.
- let it evolve unitarily without measuring it: $U|\psi\rangle$, where U is unitary.

Solving linear systems

Solving linear systems on a classical/quantum computer

Definition (Classical case)

Given access to a matrix $A \in \mathbb{R}^{n\times d}$*, and a vector* $\mathbf{b} \in \mathbb{R}^n$*, output* $A^+\mathbf{b}$ *up to error* ε*, where* A^+ *is the pseudoinverse.*

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Given the same access to a matrix $A \in \mathbb{R}^{n\times d}$, and the ability to prepare $|\mathbf{b}\rangle$, output $|A^+\mathbf{b}\rangle$ up to error ε.

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Theorem (Harrow, Hassidim, Lloyd 2008 + many others)

There is a quantum algorithm that solves this problem in cost

$$\kappa \cdot \mathrm{poly}(\log(nd), \log(1/\varepsilon)),$$

where κ is the condition number.

A comparison

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- require a classical computer to output an analogue of a quantum state (quantum-inspired classical algorithms), or
- require a quantum computer to output a vector solution

Main focus of this talk

Design a new quantum algorithm that can output vector solutions.

[5] Drineas+Mahoney '10; Mahoney '11; Drineas et al. '12

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For this problem, a naive quantum algorithm is

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Main technique: a quantum speedup of leverage score sampling,

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Main technique: a quantum speedup of leverage score sampling, an important sampling and sketching tool in randomised numerical linear algebra.[5]

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Sampling and Sketching Method

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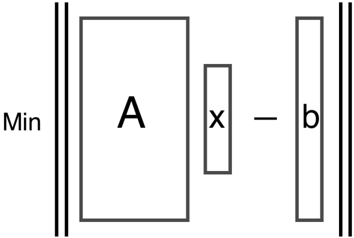
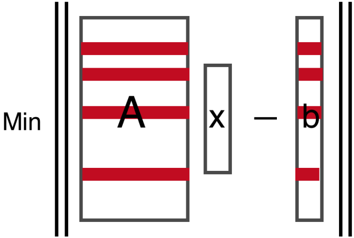
We are given a linear regression



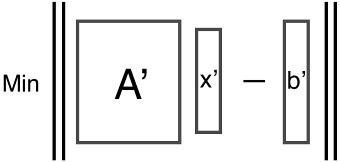
Sampling and Sketching

First, we sample some rows of $A, \mathbf{b}$ according to some distribution.



Sampling and Sketching

Then, we solve a reduced linear regression



[6] Clarkson+Woodruff '17

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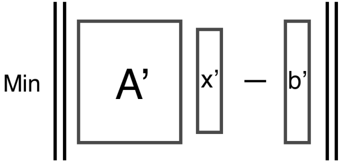

- Let $\mathbf{x}'_{\mathrm{opt}}$ be the optimal solution of the reduced problem and $\mathbf{x}_{\mathrm{opt}}$ be the optimal solution of the original problem. Then under certain conditions,

$$\|A\mathbf{x}'_{\mathrm{opt}} - \mathbf{b}\| \leq (1+\varepsilon)\|A\mathbf{x}_{\mathrm{opt}} - \mathbf{b}\|.$$

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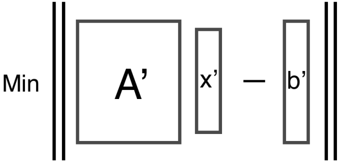

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$$\|A\mathbf{x}'_{\text{opt}} - \mathbf{b}\| \leq (1+\varepsilon)\|A\mathbf{x}_{\text{opt}} - \mathbf{b}\|.$$

- The complexity can be $O(\text{nnz}(A))$, the number of nonzero entries of A.[6]

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Leverage score sampling

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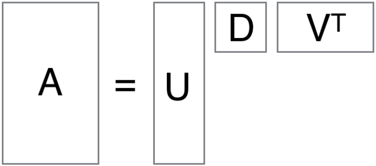
Definition (Leverage scores)

Assume $A \in \mathbb{R}^{n \times d}$ *has rank* r *and SVD*



Then the i*-th row leverage score of* A *is*

$$\mathcal{L}_i = \|U_i\|^2,$$

where U_i *is the* i*-th row of* U*.*

Some properties

1. For $\arg\min \|A\mathbf{x} - \mathbf{b}\|$, a solution is $\mathbf{x}_{\text{opt}} = (A^T A)^{-1} A^T \mathbf{b}$. Thus $\mathbf{b} \approx A\mathbf{x}_{\text{opt}} = H\mathbf{b}$, where $H = A(A^T A)^{-1} A^T$ is the so-called hat matrix. Then

$$H_{ii} = \mathcal{L}_i.$$

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$$H_{ii} = \mathcal{L}_i.$$

2. $\sum_{i=1}^{n} \mathcal{L}_i = r$, so it defines a probability distribution

$$\{p_i = \mathcal{L}_i / r : \quad i = 1, \ldots, n\}.$$

Computing all leverage scores: randomised algorithms

In [Drineas et al: arXiv:1109.3843], a randomised algorithm was proposed to approximate all leverage scores up to relative error ε in cost

$$\widetilde{O}(nd/\varepsilon^2 + d^3/\varepsilon^2).$$

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This was later improved to

$$\widetilde{O}(\mathrm{nnz}(A) + \mathrm{poly}(r/\varepsilon))$$

by Clarkson and Woodruff [arXiv:1207.6365], where

- $\mathrm{nnz}(A)$ = number of nonzero entries of A.
- r = rank of A.

Quantum Speedup of Leverage Score Sampling

Quantum speedup of leverage score sampling

In the quantum case, one way to use leverage score sampling is by preparing

$$|\mathcal{L}_A\rangle := \frac{1}{\sqrt{r}} \sum_{i=1}^{n} \sqrt{\mathcal{L}_i}\, |i\rangle.$$

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- Approximate $\mathcal{L}_i$ using amplitude estimation technique.
- We can prepare $|\mathcal{L}_A\rangle$ without computing any $\mathcal{L}_i$.

Quantum speedup of leverage score sampling

Theorem

Assume that A has rank r, and U is an α-block-encoding of A that is implemented in time $O(T)$. Then there is a quantum algorithm that prepares

$$|\mathcal{L}_A\rangle = \frac{1}{\sqrt{r}} \sum_{i=1}^{n} \sqrt{\mathcal{L}_i}\, |i\rangle$$

in time

$$\widetilde{O}\left(\mathcal{K}\sqrt{\min(n,d)/r}\right),$$

where $\mathcal{K} = T\alpha/\sigma_{\min}$ and $\sigma_{\min}$ is a lower bound of the minimal nonzero singular value of A.

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- if A is s-sparse, then $\mathcal{K} = \widetilde{O}(s\|A\|_{\max}/\sigma_{\min})$.
- if A is dense, then $\mathcal{K} = \widetilde{O}(\sqrt{nd}\|A\|_{\max}/\sigma_{\min})$.

Quantum speedup of leverage score sampling

Theorem

Make the same assumptions as above, then there is a quantum algorithm that for each j returns $\widetilde{\mathcal{L}}_j$ in time

$$\widetilde{O}(\mathcal{K}/\varepsilon)$$

such that

$$\left|\widetilde{\mathcal{L}}_j - \mathcal{L}_j\right| \leq \varepsilon\sqrt{\mathcal{L}_j}.$$

Proof sketch: block-encoding

When solving matrix-related problems, we need a way to encode the data into a quantum computer. Block-encoding is one efficient way to do this.[7]

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Definition (α-block-encoding)

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This is not always possible. It is possible for some structured matrices, e.g., sparse matrices.

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Proof sketch: quantum singular value transform[8]

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- Given $U = \begin{pmatrix} A/\alpha & * \\ * & * \end{pmatrix}$.
- Given a bounded polynomial f of degree d.
- Then there is a quantum circuit that implements the unitary

$$\widetilde{U} = \begin{pmatrix} f^{(\mathsf{SV})}(A/\alpha) & * \\ * & * \end{pmatrix},$$

where

$$f^{(\mathsf{SV})}(UDV^T) = Uf(D)V^T.$$

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- It uses $O(d)$ applications of U, U^T.

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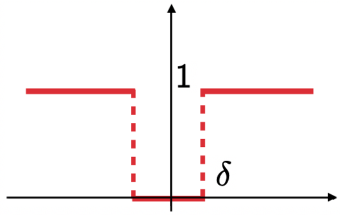
Proof sketch: An example

Suppose f is close to the rectangular function



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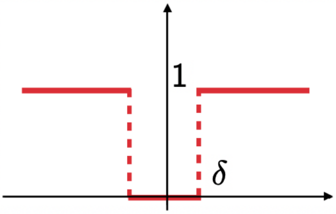

Suppose $\delta < \sigma_{\min}$, then

$$f^{(\mathsf{SV})}(UDV^T) \approx UV^T.$$

This is useful in polar decomposition.

Proof sketch: continued

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Now consider $(I \otimes W)|\phi\rangle$, where (recall $\mathbf{e}_i = |i\rangle$)

$$|\phi\rangle = \frac{1}{\sqrt{n}} \sum_{i=0}^{n-1} |i\rangle \otimes \boxed{|0\rangle \otimes |i\rangle} \qquad \begin{pmatrix} |i\rangle \\ 0 \end{pmatrix}$$

Then we obtain

$$\frac{1}{\sqrt{n}} \sum_{i=0}^{n-1} |i\rangle \otimes VU^T|i\rangle + |\perp\rangle.$$

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Then we obtain

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Since $\mathcal{L}_i = \|VU^T|i\rangle\|^2$, the first part is “equivalent” to

$$\frac{1}{\sqrt{n}} \sum_{i=0}^{n-1} \sqrt{\mathcal{L}_i}\, |i\rangle$$

if we only care about sampling.

An application to solve linear regressions

Solving linear regressions: classical

A randomised algorithm for solving linear regressions.[9]

[9] Drinea et al: 0710.1435

[10] Clarkson, Woodruff: 1207.6365

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1. Initialize $S = 0 \in \mathbb{R}^{q\times n}$, where $q = O(r/\varepsilon)$, $r = \mathrm{rank}(A)$.
2. **Approximation:**
   Approximate all the row leverage-scores $\{\mathcal{L}_i : i \in [n]\}$ of A.

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1. Initialize $S = 0 \in \mathbb{R}^{q\times n}$, where $q = O(r/\varepsilon)$, $r = \mathrm{rank}(A)$.
2. **Approximation:**
   Approximate all the row leverage-scores $\{\mathcal{L}_i : i \in [n]\}$ of A.
3. **Sampling:**
   Sampling according to $\{\mathcal{L}_i/r : i \in [n]\}$, if i is sampled, then set the i-th row of S as $\mathbf{e}_i^T/\sqrt{qp_i}$, where $\{\mathbf{e}_1, \ldots, \mathbf{e}_n\}$ is the standard basis of $\mathbb{R}^n$.

[9] Drinea et al: 0710.1435

[10] Clarkson, Woodruff: 1207.6365

Solving linear regressions: classical

A randomised algorithm for solving linear regressions.[9]

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The main cost comes from the second step of computing all leverage scores, which is $\widetilde{O}(\mathrm{nnz}(A) + r^3)$.[10]

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3. **Approximation:**
   Approximate $p_j = \mathcal{L}_j/r$ for all $j \in J$ up to a small constant relative error. Denote the results as $\tilde{p}_j$, set the j-th row of S as $\mathbf{e}_j^T/\sqrt{q\tilde{p}_j}$.

Comparison

	Complexity (of finding S)
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When A is sparse and low-rank, then in the worst case

$$\mathsf{nnz}(A) = n + d, \quad \mathcal{K}\sqrt{n} = s\sqrt{n}\,\|A\|_{\max}/\sigma_{\min}.$$

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$\Rightarrow$ Quadratic speedup, may have superpolynomial speedup when $\mathcal{K} \ll n + d$.

Outlook

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Thanks very much for your attention!

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