Quantum-inspired ℓ^2 sampling

and applications to machine learning

Faris Sbahi

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Machine Learning

Quantum Machine Learning

Classical ℓ^2 sampling

Remarks

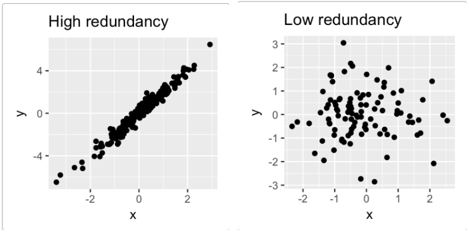
Machine Learning
Introduction

- Machine learning is a broad term for algorithms which are capable of finding patterns in data.
- Fundamental goal: capture these patterns in a "model" that *generalizes* to unseen data.
- These algorithms have two components:
    1. A learning element. Updates the model depending on its performance on the considered dataset.
    2. A performance element. Provides the measure of performance.
- Bottom line: "machine learning" is a somewhat hollow term. Many ML algorithms are in fact familiar linear algebraic techniques.

PCA

Motivation: Singular value transformation

- "Training" dataset $\mathcal{T}$ consists of the accessible samples of data. $\mathcal{T}$ is drawn from a subset of $\Omega \subset \mathbb{R}^d$ where each component represents a "feature".
- Samples from Ω are assumed to be drawn according to some distribution $\mathcal{D}$.
- Example: data is collected on the heights and lengths of cherry blossom petals.

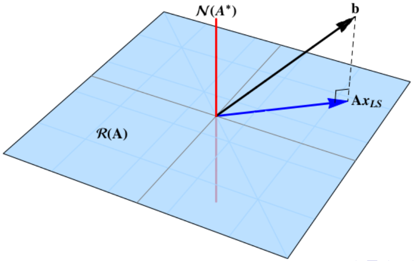


- How and why may it make sense to reduce the dimensionality of the feature space?

Moore-Penrose Pseudoinverse

Motivation: Singular value transformation

- Let $A \in \mathbb{R}^{m \times n}$ and $b \in \mathbb{R}^m$ unit vector. In machine learning, A is the matrix with rows given by the samples of $\mathcal{T}$. We assume the distribution $\mathcal{D}$ now extends to $\Omega \times Y$, $Y \subset \mathbb{R}$.
- We wish to find the x_{LS} which satisfies $x_{LS} = \arg\min_x \|Ax - b\|_2$
- Notation: $x_{LS} = A^+ b$
- Common strategy uses SVD: write $A = UDV^\dagger$ and then $A^+ = VD^+U^\dagger$ where D^+ simply inverts the non-zero diagonal entries.



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Moore-Penrose Pseudinverse

Harrow, Hassidim, Lloyd (orig.) Wiebe, Braun

- HHL algorithm: application of phase estimation and Hamiltonian simulation to solve linear system.
- We can use HHL as a subroutine to compute $A^+ |b\rangle = |x\rangle$ in ($|x\rangle$ is the least-square solution).
- Note that $|x\rangle$ is a quantum state. Hence, we may efficiently measure an expectation value $x^T Mx$ where M is some p.s.d operator.
- Runtime bound $\tilde{O}(log(N)(s^3\kappa^6)/\epsilon)$ time (query complexity)
- Assumption: A is sparse with low condition number κ. Hamiltonian ($\hat{H}$) simulation is efficient when $\hat{H}$ is sparse. No low-rank assumptions are necessary.
- "Key" assumption: the quantum state $|b\rangle$ can be prepared efficiently.

Read the Fine Print

- In general QML algorithms convert quantum input states to the desired quantum output state.
- In practice, data is initially stored classically and the algorithm's output must be accessed classically as well.
- This poses two problems if seek to use these algorithms: the "state preparation" and "readout" problems.
- Even if we ignore the readout problem, can we at least find a state preparation routine that maintains a speedup for the discussed quantum algorithms? Open question!
- See "Quantum Machine Learning Algorithms: Read the Fine Print" by Aaronson

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In search of a "fair" comparison

- How can we compare the speed of quantum algorithms with quantum input and quantum output to classical algorithms with classical input and classical output?
- Quantum machine learning algorithms can be exponentially faster than the best standard classical algorithms for similar tasks, but this comparison is unfair because the quantum algorithms get outside help through input state preparation.
- We want a classical model that helps its algorithms stand a chance against quantum algorithms, while still ensuring that they can be run in nearly all circumstances one would run the quantum algorithm.
- Solution (Tang): compare quantum algorithms with quantum state preparation to classical algorithms with sample and query access to input.

Classical ℓ^2 Sampling Model

Definition
We have "query access" to $x \in \mathbb{C}^n$ if, given $i \in [n]$, we can efficiently compute x_i. We say that $x \in \mathcal{Q}$.

Definition
Definition. We have sample and query access to $x \in \mathbb{C}^n$ if we have query access to x; can produce independent random samples $i \in [n]$ where we sample i with probability $|x_i|^2/\|x\|^2 x$ and can query for $\|x\|$. We say that $x \in \mathcal{SQ}$.

Definition
Definition. For $A \in \mathbb{C}^{m \times n}$, $A \in \mathcal{SQ}$ (abuse) iff $A_i \in \mathcal{SQ}$ for A_i the rows of A, along with $\tilde{A} \in \mathcal{SQ}$ for $\tilde{A}$ the vector of row norms (so $\tilde{A}_i = \|A_i\|$).

"Dequantization" (Tang)

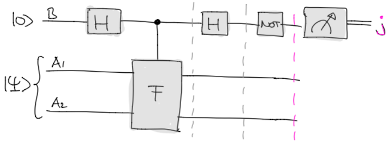
Definition

Let $\mathcal{A}$ be a quantum algorithm with input $|\varphi_1\rangle, \ldots, |\varphi_C\rangle$ and output either a state $|\psi\rangle$ or a value λ. We say we dequantize $\mathcal{A}$ if we describe a classical algorithm that, given $\varphi_1, \ldots, \varphi_C \in \mathcal{SQ}$, can evaluate queries to $\psi \in \mathcal{SQ}$ or output λ, with similar guarantees to $\mathcal{A}$ and query complexity poly(C).

Dequantization Toolbox

Method 1: Inner product estimation (Tang, 2018)

- For $x, y \in \mathbb{C}^n$, if we are given that $x \in \mathcal{SQ}$ and $y \in \mathcal{Q}$, then we can estimate $\langle x, y \rangle$ with probability $\geq 1 - \delta$ and error $\epsilon \|x\| \|y\|$
- Quantum analogue: SWAP test



Dequantization Toolbox

Method 1: Inner product estimation (Tang, 2018)

Fact

For $\{X_{i,j}\}$ i.i.d random variables with mean μ and variance σ^2, let

$$Y := \underset{j \in [6 \log 1/\delta]}{\text{median}} \ \underset{i \in [6/\epsilon^2]}{\text{mean}} \ X_{i,j}$$

Then $|Y - \mu| \leq \epsilon\sigma$ with probability $\geq 1 - \delta$, using only $O(\frac{1}{\epsilon^2} \log \frac{1}{\delta})$ copies of X.

Proof.

(sketch) The proof follows from two facts:

- first, the median of $C_1, \ldots, C_n$ is at least λ precisely when at least half of the C_i are at least λ;
- second, Chebyshev's inequality (applied to the mean).

$\square$

Dequantization Toolbox

Method 1: Inner product estimation (Tang, 2018)

Corollary

For $x, y \in \mathbb{C}^n$, given $\mathcal{SQ}(x)$ and $\mathcal{Q}(y)$, we can estimate $\langle x, y \rangle$ to $\epsilon \|x\| \|y\|$ error with probability $\geq 1 - \delta$ with query complexity $O(\frac{1}{\epsilon^2} \log \frac{1}{\delta})$

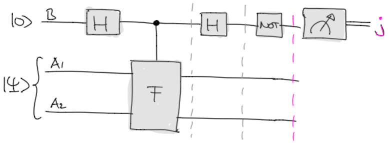
Proof.

Sample s from v and let $Z = x_s v_s \frac{\|v\|^2}{|v_s|^2}$. Apply the Fact with $X_{i,j}$ being independent copies of Z. □

Dequantization Toolbox

Method 2: Thin Matrix-Vector (Tang, 2018)

- For $V \in \mathbb{C}^{n\times k}$, $w \in \mathbb{C}^k$, given $V^\dagger \in \mathcal{SQ}$ (i.e. column-wise of V) and $w \in \mathcal{Q}$, we can simulate $Vw \in \mathcal{SQ}$ with poly(k) queries
- Quantum analogue: SWAP test



Dequantization Toolbox

Method 2: Thin Matrix-Vector (Tang, 2018)

Definition

Rejection sampling

Algorithm

Input: Samples from distribution P

Output: Samples from distribution Q

- *Sample s from P*
- *Compute $r_s = \frac{1}{M}\frac{Q(s)}{P(s)}$*
- *Output s with probability r_s and restart otherwise*

Fact

Fact. If $r_i \leq 1, \forall i$, then the above procedure is well-defined and outputs a sample from Q in M iterations in expectation.

Dequantization Toolbox

Method 2: Thin Matrix-Vector (Tang, 2018)

Proposition

For $V \in \mathbb{R}^{n\times k}$ and $w \in \mathbb{R}^k$, given $V \in \mathcal{SQ}$ and $w \in \mathcal{Q}$, we can simulate $Vw \in \mathcal{SQ}$ with expected query complexity $O(k^2 C(V,w))$, where

$$C(V,w) := \frac{\sum_{i=1}^{k} \|w_i V^{(i)}\|^2}{\|Vw\|^2}$$

We can compute entries $(Vw)_i$ with $O(k)$ queries.
We can sample using rejection sampling:

- *P is the distribution formed by sampling from $V^{(j)}$ with probability proportional to $\|w_j V^{(j)}\|^2$*
- *Q is the target Vw.*

$$r_i = \frac{(Vw)_i^2}{k\sum_{j=1}^{k}(w_j V_{ij})^2} = \frac{Q(i)}{kC(V,w)P(i)}$$

Dequantization Toolbox

Method 2: Thin Matrix-Vector (Tang, 2018)

- Notice that we can compute these r_i's (in fact, despite that we cannot compute probabilities from the target distribution), and that the rejection sampling guarantee is satisfied (via Cauchy-Schwarz).
- The probability of success is $\frac{\|Vw\|^2}{k\sum_{i=1}^{k}\|w_i V^{(i)}\|^2}$. Thus, to estimate the norm of Vw, it suffices to estimate the probability of success of this rejection sampling process.
- Through a Chernoff bound, we see that the average of $O(kC(V,w)(\frac{1}{\epsilon^2}\log\frac{1}{\delta}))$ "coin flips" is in $[(1-\epsilon)\|Vw\|,(1+\epsilon)\|Vw\|]$ with probability $\geq 1-\delta$, where each coin flip costs k queries and samples.

Dequantization Toolbox

Method 3: Low-Rank Approximation (Frieze, Kannan, Vempala, 1998)

- For $A \in \mathbb{C}^{m \times n}$, given $A \in \mathcal{SQ}$ and some threshold k, we can output a description of a low-rank approximation of A with $\text{poly}(k)$ queries.
- Specifically, our output is $\mathcal{SQ}(S, \hat{U})$ for $S \in \mathbb{C}^{\ell \times n}$, $\hat{U} \in \mathbb{C}^{\ell \times k}$ ($\ell = \text{poly}(k, \frac{1}{\epsilon})$), and this implicitly describes the low-rank approximation to A, $D := A(S^\dagger \hat{U})(S^\dagger \hat{U})^\dagger$ (notice rank $D \leq k$).
- This matrix satisfies the following low-rank guarantee with probability $\geq 1 - \delta$: for $\sigma := \sqrt{2/k}\|A\|_F$, and $A_\sigma := \sum_{\sigma_i \geq \sigma} \sigma_i u_i v_i^\dagger$ (using SVD),
$$\|A - D\|_F^2 \leq \|A - A_\sigma\|_F^2 + \epsilon^2 \|A\|_F^2$$
- This guarantee is non-standard: instead of A_k, we use A_σ. This makes our promise weaker, since it is useless if A has no large singular values.
- Quantum analogue: phase estimation

Moore-Penrose Pseudoinverse (low-rank)

Application

Problem

For a low-rank matrix $A \in \mathbb{R}^{m \times n}$ and a vector $x \in \mathbb{R}^n$, given $x, A \in \mathcal{SQ}$, (approximately) respond to requests for $A^+ x \in \mathcal{SQ}$, where A^+ is the pseudoinverse of A.

Algorithm

- *Use the low-rank approximation protocol (3) to get $\mathcal{SQ}(S, \hat{U})$.*
- *From applying the matrix-vector protocol (2), we have $\mathcal{SQ}(\hat{V})$, where $\hat{V} := S^T \hat{U}$; we can show that the columns of $\hat{V}$ behave like the right singular vectors of A.*
- *Further, (3) also outputs their approximate singular values $\hat{\sigma}_i$*
- *Hence, we can approximate the vector we wish to sample:*

$$A^+ x = (A^T A)^+ A^T x \approx \sum_{i=1}^{k} \frac{1}{\hat{\sigma}_i^2} \hat{v}_i \hat{v}_i^T A^T x$$

Moore-Penrose Pseudoinverse (low-rank) cont.

Application

- We approximate $\hat{v}_i^T A^T x$ to additive error for all by noticing that $\hat{v}_i^T A^T x = \mathrm{Tr}\big(A^T x \hat{v}_i^T\big)$ is an inner product of the order two tensors $A^T A$ and $x \hat{v}_i^T x$.
- Thus, we can apply (1), since being given $\mathcal{SQ}(A)$ implies $\mathcal{SQ}(A^T)$ for $A^T A$ viewed as a long vector.
- Finally, using (2), sample from the linear combination using these estimates and $\hat{\sigma}_i$.

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Thoughts

- Conjecture: For machine learning problems, SQ assumptions are more reasonable than state preparation assumptions.
- We discussed pseuo-inverse which inverts singular values, but in principle we could have applied any function to the singular values
- Gilyen et. al (2018) show that many quantum machine learning algorithms indeed apply polynomial functions to singular values
- Our discussion suggests that exponential quantum speedups are tightly related to problems where high-rank matrices play a crucial role (e.g. Hamiltonian simulation or QFT)