Householder Sketch for Accurate and Accelerated Least-Mean-Squares Solvers

ICML 2021

Jyotikrishna Dass Rabi Mahapatra

{dass.jyotikrishna,rabi}@tamu.edu

Department of Computer Science and Engineering



 $| \operatorname{TEXAS}_{U \ N \ I \ V \ E \ R} A \& M_{I \ V} |$

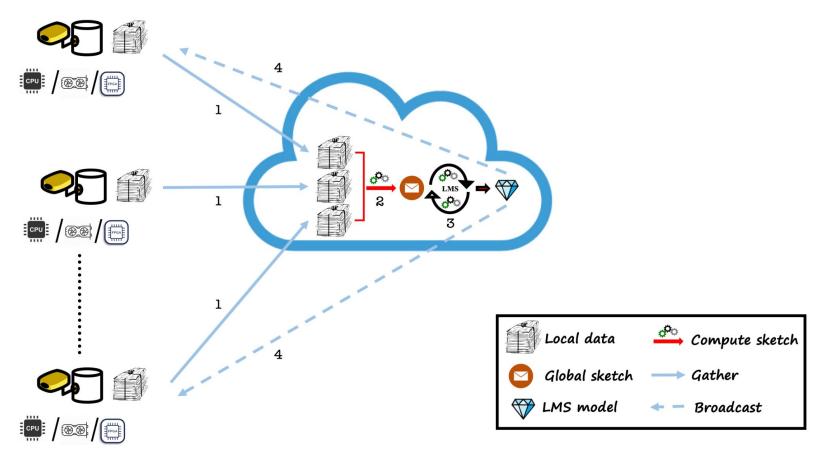
Sketching

A compressed mapping of few or all data points (*X*) in a data set to generate **data summary** called *Sketch* (*S*) to preserve or approximate the covariance matrix, i.e.,

$S^T S \cong X^T X$



Sketch-based ML Framework





Least-Mean-Squares (LMS)

$$\min_{\mathbf{w}} f(\|\mathbf{X}\mathbf{w}-\mathbf{y}\|_2) + g(\mathbf{w}).$$

LINEAR REGRESSION, $f(z) = z^2$, and $g(\mathbf{w}) = 0$.

 $(\mathbf{X}^T\mathbf{X})\mathbf{w} = \mathbf{X}^T\mathbf{y}$

RIDGE REGRESSION, $f(z) = z^2$, and $g(\mathbf{w}) = \lambda ||\mathbf{w}||_2$, where, $\lambda > 0$, $(\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I})\mathbf{w} = \mathbf{X}^T \mathbf{y}$

Our focus is on theoretically accurate summary of input data which could be directly plugged to accelerate scikit-learn LMS solvers



Inspiration

(Maalouf et al.)¹ proposed LMS-BOOST

- Coreset-Sketch fusion algorithm
- Faster implementation of Caratheodory Theorem (1907)
- Accurately solve and accelerate LMS solvers in scikit-learn library upto 100x
 - summarizes input data $\boldsymbol{\mathcal{X}}$ into matrix $\boldsymbol{\mathcal{S}}$ of size $\boldsymbol{O}(d^2) \times d$
 - preserves the input covariance, i.e. $S^T S = X^T X$
 - computational time complexity of $O(nd^2 + log(n) \times d^8)$

Claim 1: QR decomposition is relatively time-consuming.

Claim 2: QR decomposition is unsuitable for exact factorization for streaming data.

¹Maalouf, A., Jubran, I., and Feldman, D. "*Fast and accurate least-mean-squares solvers*". in Advances in Neural Information Processing Systems, pp. 8305–8316, 2019



Contributions

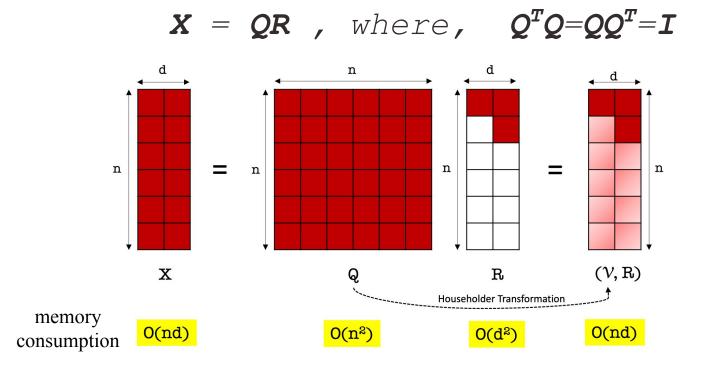
Test and Check validity of the above claims made against the QR decomposition as a candidate for data summary via extensive theoretical and empirical analysis

- **Q1:** Whether a classical and simple approach such as QR decomposition could (theoretically) accurately solve and accelerate common LMS solvers compared to the above state of the art recursive and clustering-based fusion algorithm?
- **Q2:** Whether a numerically stable algorithm could generate accurate distributed sketches via exact factorization on streaming data?



Householder-QR

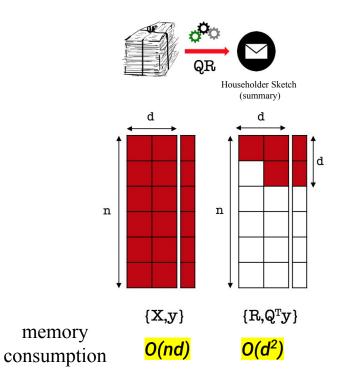
Theorem 2.1 (Householder-QR (Golub & Van Loan, 2012)). Let matrix $X \in \mathbb{R}^{n \times d}$ with n > d. Householder QR decomposition of X generates set of d Householder matrices \mathcal{H} and an $n \times d$ upper trapezoidal matrix R. The Householder matrices are stored as a set of d Householder reflectors \mathcal{V} . Total memory footprint of above factors is nd elements with time complexity of $O(nd^2)$ for $n \gg d$.





Householder Sketch

Theorem 2.2 (Householder Sketch). Let $X \in \mathbb{R}^{n \times d}$ be the original data matrix, $y \in \mathbb{R}^n$ be the corresponding output label or response vector, and $n \gg d$. Let X = QR be Householder QR decomposition. Then, $(R, Q^T y)$ is a memory-efficient and theoretically accurate sketch of original data (X, y) such that $X^T X = R^T R$, and has memory footprint of $\left(\frac{d(d+3)}{2}\right)$ elements, computed in time $O(nd^2)$.





Householder Sketch for LMS

Least-Mean-Squares

$$\min_{\mathbf{w}} f(\|\mathbf{X}\mathbf{w}-\mathbf{y}\|_2) + g(\mathbf{w}).$$

$$\min_{\mathbf{w}} f(\|\mathbf{Q}\mathbf{R}\mathbf{w}-\mathbf{y}\|_2) + g(\mathbf{w}).$$

$$\|\mathbf{X}\mathbf{w} - \mathbf{y}\|_{2} = \|\mathbf{Q}\mathbf{R}\mathbf{w} - \mathbf{y}\|_{2} = \|\mathbf{Q}\mathbf{R}\mathbf{w} - \mathbf{Q}\mathbf{Q}^{T}\mathbf{y}\|_{2} = \|\mathbf{Q}\|_{2} \|\mathbf{R}\mathbf{w} - \mathbf{Q}^{T}\mathbf{y}\|_{2} = \|\mathbf{R}\mathbf{w} - \mathbf{Q}^{T}\mathbf{y}\|_{2}$$
(LMS)

$$Accurate Sketch$$

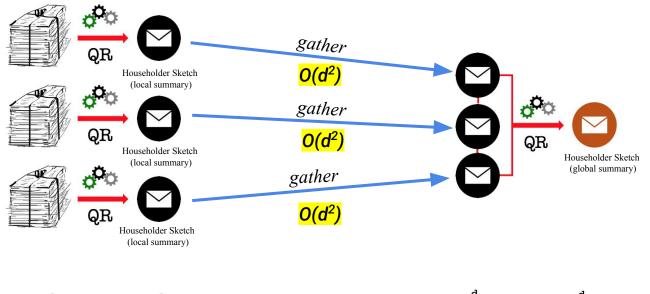
$$R^{T}R = X^{T}X$$

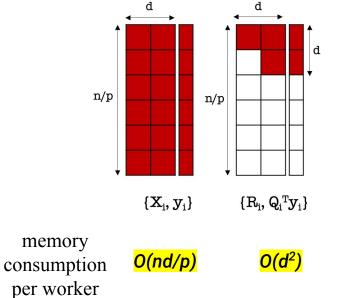
Distributed Householder Sketches

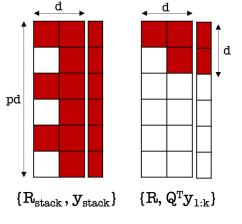
Theorem 3.1 (Distributed Householder-QR (Dass et al., 2018)). Let $X = (X_1^T | \dots | X_p^T)^T$, where, $X_i \in \mathbb{R}^{\hat{n} \times d}$ be local data matrix of parallel worker, $i = 1, \dots, p$, where $\hat{n} \gg d$, and, $n = p\hat{n}$. Let, $X_i = Q_i R_i$ be constructed via local HOUSEHOLDER-QR (see Algorithm 1) for each $i = 1, \dots, p$, in parallel. Then, X = QR for the complete data matrix can be constructed exactly, such that $Q = \text{diag}(Q_1, \dots, Q_p)Q_M$, and $R = R_M$, where $R_{stack} = Q_M R_M$ via another HOUSEHOLDER-QR on $R_{stack} = (R_1^T | \dots | R_p^T)^T$ gathered from all workers. The above DISTRIBUTED HOUSEHOLDER-QR has a computational time complexity of $O(\frac{n}{p}d^2)$, with a communicated data volume of $(\frac{d(d+1)}{2})$ elements by each worker.

$$\mathbf{X} = \begin{pmatrix} \mathbf{X}_1 \\ \mathbf{X}_2 \\ . \\ . \\ . \\ \mathbf{X}_p \end{pmatrix} = \begin{pmatrix} \mathbf{Q}_1 \mathbf{R}_1 \\ \mathbf{Q}_2 \mathbf{R}_2 \\ . \\ . \\ . \\ \mathbf{Q}_p \mathbf{R}_p \end{pmatrix} = \operatorname{diag}(\mathbf{Q}_1, \dots, \mathbf{Q}_p) \begin{pmatrix} \mathbf{R}_1 \\ \mathbf{R}_2 \\ . \\ . \\ \mathbf{R}_p \end{pmatrix} , \qquad \mathbf{R}_{stack} = \begin{pmatrix} \mathbf{R}_1 \\ \mathbf{R}_2 \\ . \\ . \\ \mathbf{R}_p \end{pmatrix} = \mathbf{Q}_M \mathbf{R}_M$$

$$\mathbf{X} = \text{diag}(\mathbf{Q}_1, \dots, \mathbf{Q}_p) \mathbf{R}_{stack} = \text{diag}(\mathbf{Q}_1, \dots, \mathbf{Q}_p) \mathbf{Q}_M \mathbf{R}_M$$
R







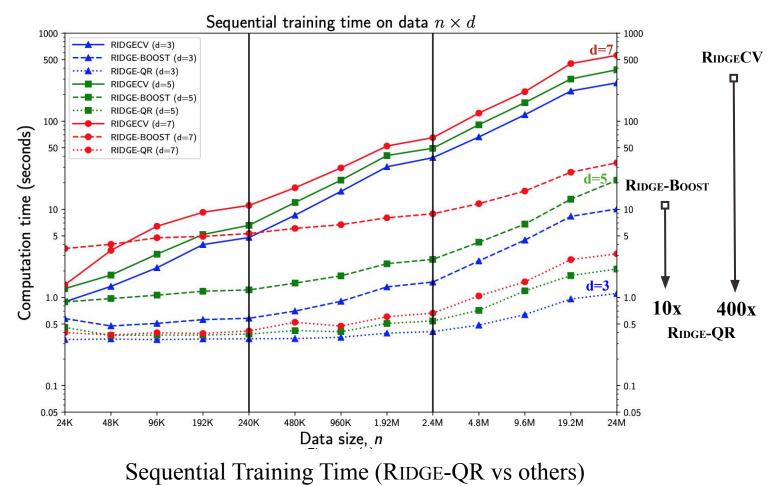
<mark>0(d²)</mark>

p: #workers

<mark>O(pd²)</mark>

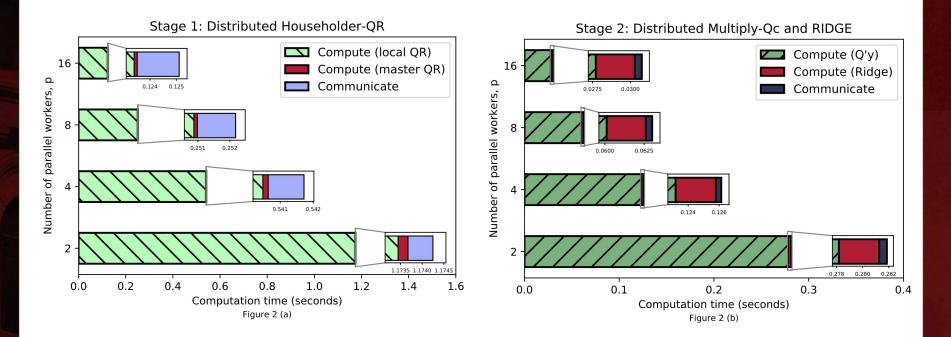


Results (1/3)





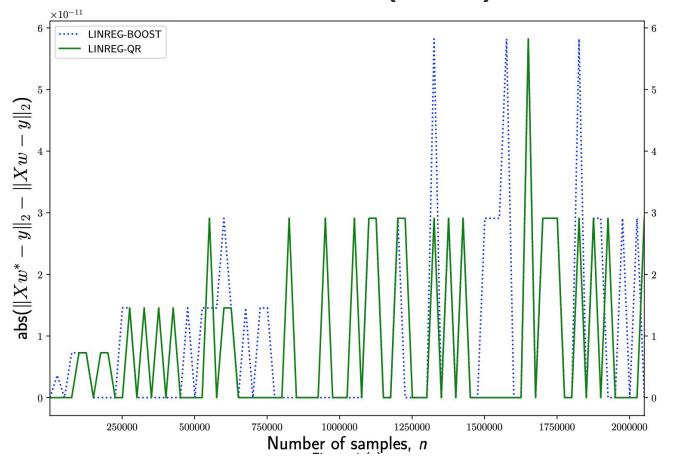
Results (2/3)



Execution Time breakdown of DISTRIBUTED RIDGE-QR (on 10M x 10) with zoomed insets depicting communication time



Results (3/3)



Accuracy (×10⁻¹¹) comparison of LINREG-QR and LINREG-BOOST on Household Power Consumption dataset (~ $2M \times 8$), w* is solution from scikit-learn *LinearRegression*



Conclusions

Claim 1: QR decomposition is relatively time-consuming FALSE

→ Householder sketch is more memory-efficient and accelerates common LMS solvers in scikit-learn library up to 100x-400x, and outperforms the strong baseline LMS- BOOST by 10x-100x with similar numerical stability.

Claim 2: QR decomposition is unsuitable for exact factorization for streaming data FALSE

→ The distributed implementation generates accurate distributed sketches and achieves linear scalability with negligible communication overhead for large sample size and dimension across multiple worker nodes.









