Parallel and Communication Avoiding Least Angle Regression

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Abstract

We are interested in parallelizing the Least Angle Regression (LARS) algorithm for fitting linear regression models to high-dimensional data. We consider two parallel and communication avoiding versions of the basic LARS algorithm. The two algorithms apply to data that have different layout patterns (one is appropriate for row-partitioned data, and the other is appropriate for column-partitioned data), and they have different asymptotic costs and practical performance. The first is bLARS, a block version of LARS algorithm, where we update b columns at each iteration. Assuming that the data are row-partitioned, bLARS reduces the number of arithmetic operations, latency, and bandwidth by a factor of b. The second is Tournament-bLARS (T-bLARS), a tournament version of LARS, in which case processors compete, by running several LARS computations in parallel, to choose b new columns to be added into the solution. Assuming that the data are column-partitioned, T-bLARS reduces latency by a factor of b. Similarly to LARS, our proposed methods generate a sequence of linear models. We present extensive numerical experiments that illustrate speed-ups up to 25x compared to LARS.

1 Motivation and outline

Recently there has been large growth in data for many applications in statistics, machine learning and signal processing and this poses the need for powerful computer hardware as well as new algorithms that utilize the new hardware efficiently. Commercial hardware companies started to construct multicore designs because the performance of single central processing units (CPUs) is stagnating due to heat issues, i.e., “the Power Wall” problem [30]. In terms of software and algorithm implementations for processing large-scale data, the increased number of cores might require synchronization among them and this results in data transfer between levels of a memory hierarchy or between CPUs over a network. For this reason the total running time of a parallel algorithm depends on the number of arithmetic operations (computational costs) and the cost of data movement (communication costs). The communication cost includes the “bandwidth cost”, i.e. the number of bytes, or more abstractly, number of words, sent among cores for synchronization purposes, and the “latency cost”, i.e. the number of messages sent. On modern computer architectures, communicating data often takes much longer than performing a floating-point operation and this gap is continuing to increase [34]. Therefore, it is especially important to design algorithms that minimize communication in order to attain high performance on modern computer architectures.

In this paper we will propose two novel parallel and communication avoiding versions of the least angle regression algorithm which is a very popular method for sparse linear regression [16]. A plethora of applications in statistics [16], machine learning [28] and signal processing/compressed sensing [4] utilize sparse linear models. To the best of our knowledge there is no study on parallelizing LARS.

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2 Introduction to the problem, existing models and LARS

Let $A \in \mathbb{R}^{m \times n}$ be a data matrix with $m$ samples and $n$ features. We are concerned with the problem of finding a vector $y := Ax$ that approximates a given vector $b \in \mathbb{R}^m$, where vector $y$ is a linear combination of a few columns/features of the given data matrix $A$. This means that we are looking for a coefficients vector $x$ that is sparse, i.e., it has few number of non-zeros.

Over the years there have been proposed many algorithms/models to solve this problem. In what follows, we review the ones that to the best of our knowledge are the most important. There are two main categories of algorithms/models to solve this problem. The first category consists of algorithms that progressively select a subset of columns/features based on their absolute correlation with the residual vector $y - b$. In particular, the classic Forward Selection algorithm in Section 8.5 in [39] selects the first column/feature with the largest absolute correlation with the response $b$. Let's denote the index of the selected column with $i$, the corresponding column with $A_i$ and the corresponding coefficient $x_i$. The next step of the algorithm is to solve a simple linear regression problem

$$\min \frac{1}{2} \| A_i x_i - b \|_2^2.$$  

By solving this simple regression problem we obtain the value of the optimal coefficient $x_i$. The residual $r := Ax_i - b$, which is orthogonal to $A_i$, is now considered the new response vector for the next iteration. Finally, we project orthogonally the remaining columns in $A$ to $A_i$. Then we have to repeat this process and find a new column/feature. After $k$ iterations we will have selected $k$ columns, which we can now use to solve smaller ordinary regression problem using the response vector $b$. According to [16], in practice the Forward Selection algorithm might be aggressive in terms of selecting features since other columns might be correlated with the selected column $A_i$ that we ignored. Another algorithm in this category is the Forward Stagewise algorithm [18, 19], which in comparison to Forward Selection is much more cautious algorithm since it requires much more steps to converge to a $k$-sparse model, i.e., $k$ selected columns. More precisely, at each iteration of the Forward Stagewise we select the column that is most correlated with the current residual and we increment the corresponding coefficient in the vector $x$ by a small amount $\pm \varepsilon$, where the sign is determined based on the sign of the correlation. The small increment of elements in $x$ at each iteration is what distinguishes Forward Stagewise and Forward Selection.

The second category of models is optimization based, meaning that we solve a predefined optimization problem to obtain a sparse linear model. There are two subclasses of optimization problems in this category, the first is known as $\ell_1$-regularized linear regression or least absolute shrinkage and selection operator (LASSO) [37], the second is $\ell_0$-regularized variants. Let us first define the $\ell_1$ and $\ell_0$ norms and then we will continue with presenting the optimization problems. The $\ell_1$ norm of a vector $x$ is defined as $\|x\|_1 := \sum_{i=1}^{n} |x_i|$, while the $\ell_0$ norm is defined as $\|x\|_0 := \{\text{number of non-zero elements in } x\}$. Equipped with these definitions we define LASSO

$$\begin{array}{ll}
\text{minimize} & \frac{1}{2} \| Ax - b \|_2^2 \\
\text{subject to} & \|x\|_1 \leq \lambda,
\end{array}$$

where $\lambda$ is a model parameter. LASSO is a convex optimization problem and can be solved in polynomial time, we discuss several serial and parallel algorithms later in this paper. The LASSO optimization problem is likely to have a set of sparse optimal solutions due to the sparsity inducing $\ell_1$-ball constraint. For details we refer the reader to [37]. A non-convex alternative of LASSO, but with a direct constraint on the sparsity of $x$ is the $\ell_0$-regularized linear regression problem

$$\begin{array}{ll}
\text{minimize} & \frac{1}{2} \| Ax - b \|_2^2 \\
\text{subject to} & \|x\|_0 \leq \tau,
\end{array}$$

where $\tau$ is a model parameter that bounds the number of non-zeros in $x$. This is an NP-hard problem, however, we can find local solutions by variants of gradient descent, which we discuss later in this paper.

An important difference between the two approaches, i.e., Forward Selection or Stagewise vs LASSO, is that with the former one obtains a sequence of solutions $x_k$ with increasing number of non-zeros, while the latter we obtain a solution path $x(\lambda)$. There is a question regarding how those two solution paths defer in terms of the selected features. The LARS algorithm is an algorithmic framework that unifies those two approaches. In particular, the LARS algorithm has been motivated by the Forward Selection and Stagewise algorithms, therefore
in terms of steps it is similar to those as we will see later, but it is also proved in Theorem 1 in [16] that a certain version of LARS produces a sequence of solutions $x_k$ that is equivalent to the solution path $x(\lambda)$. Let us now summarize the steps of the LARS algorithm. This algorithm is discussed in detail in Section 6. Similarly to Forward algorithms, at the first iteration of LARS we initialize the algorithm by selecting the column with the largest absolute correlation with vector $b$. The next step is to update vector $y$. Instead of solving a simple regression problem like in Forward Selection (which is an aggressive strategy) or making $\epsilon$ updates to $x$ (which is too cautious), we define a vector $u$ that is equiangular with all previous chosen columns and then we update $y := y + u\gamma$. The step-size $\gamma \in \mathbb{R}$ is set such that the new column to be added in the next iteration has the same correlation with the new residual vector as with all other selected columns so far. This process might sound complicated at first but we will revisit the linear algebra behind these decisions in Section 6.

## 3 Our contributions

Although there are numerous parallel optimization algorithms for $\ell_0$- and $\ell_1$-regularized regression, we are not aware of any parallel and communication avoiding versions for LARS. To the best of our knowledge the proposed algorithms are the first parallel versions of LARS that are also communication avoiding. Let us briefly describe the proposed algorithms and the most significant ideas that had to be developed to establish them.

The first method is a block version of LARS which is described in Section 7. Instead of adding one feature at each iteration in the solution set we add $b$ features at a time. By blocking operations and by partitioning the data per row we are able to show that we decrease the arithmetic, latency and bandwidth costs by a factor of $b$. Extensive numerical experiments in Section 10 illustrate significant speedups for block LARS without compromising the quality of the output compared to LARS. In the same section we study empirically the trade-off between the size of $b$ and the quality of the output compared to LARS.

Careful modification of the linear algebra had to be performed in order to successfully generalize LARS to the block case and also guarantee that all steps of the algorithm are well-defined. More precisely, LARS has two important properties that we had to relax. The first is that all chosen columns at each iteration have the same absolute correlation with the residual and also they are maximally correlated. The second property is that the direction $u$ is equiangular and also has maximal correlation with the chosen columns. Block LARS maintains the property that the chosen columns at each iteration are maximally correlated but they are not equal, meaning that there is no column that hasn’t been selected with larger absolute correlation with the residual than the selected ones. Block LARS also relaxes the second property in the sense that $u$ is not equiangular with all chosen columns but it is maximally correlated, i.e., there is no column that hasn’t been selected with larger correlation than the selected ones. We show that block LARS at each iteration reduces the correlations for all selected columns similarly to LARS. Finally, if we set $b = 1$ then block LARS reduces to LARS.

The second method is a tournament block LARS method. In this method the data are partitioned per column and distributed to processors. Then each processor calls a modified version of the LARS algorithm on its local data. Each processor can run the modified LARS algorithm for $b$ iterations so that $b$ columns are chosen at termination of the local call to LARS. Using a generalized tree-reduction operation each processor/node sends its chosen columns to the parent node (starting from the bottom of the tree). The parent node calls again the modified LARS algorithm by utilizing only the columns that have been sent from the child nodes. This process repeats until we reach the root node where the final output is used to update the current vector $y$ and current set of selected columns. By partitioning the data per column (as opposed to per row for block LARS) and using the generalized tree-reduction we allow the nodes to work in parallel in local data and this way we reduce latency by a factor of $b$. Note that by setting $b = 1$ we recover the original LARS algorithm. Many of the properties of the LARS algorithm are not satisfied at a global level but some of them are maintained during the local calls to LARS. We discuss details in Section 8. In Section 10 we show that tournament block LARS can be faster than the original LARS without compromising the quality of the output. Similarly to block LARS we study the trade-off of speed and quality of output as we vary parameter $b$ and the number of processors.

## 4 Literature review for parallel models and methods

The dependence of the running time of parallel methods on communication requirements gave a totally new perspective on how to efficiently parallelize existing algorithms. Communication-avoiding algorithms became
a very popular subject of study and it has been demonstrated that such algorithms exhibit large speedups on modern, distributed- and shared-memory parallel architectures through careful algorithmic modifications [3]. Many iterative methods for linear systems and matrix decomposition algorithms have been re-organized to avoid communication and this has led to significant performance improvements over existing state-of-the-art libraries [2, 3, 6, 20, 35, 40].

The origins of communication-avoiding algorithms lie in the s-step conjugate gradients method [38] by Van Rosendale’s and in the work of Chronopoulouos on parallel iterative methods for linear systems [8]. More precisely, Chronopoulouos and Gear developed s-step methods for symmetric linear systems [10, 11], Chronopoulouos and Swanson developed s-step methods for unsymmetric linear systems [9] and Kim and Chronopoulouos developed s-step non-symmetric Lanczos method [22]. Furthermore, Demmel, Hoemmen, Mohiyuddin, and others [14, 20, 24, 25] introduced the matrix powers kernel optimization which reduces the communication cost of the s Krylov basis vector computations by a factor $O(s)$ for well-partitioned matrices. Finally, Carson, Demmel, Hoemmen developed communication-avoiding Krylov subspace methods [6, 14, 20] by combining the matrix powers kernel and s-step methods.

The above results are mainly focused on iterative methods for least-squares and linear systems. Our focus on this paper is sparse linear regression where we also require the coefficients of the model to be sparse. As is mentioned in Section 2 there are two categories of methods that can solve this problem efficiently. The first is LARS-type algorithms. To the best of our knowledge there are no studies on parallelizing LARS. However, we will see in Section 7 that the computational bottleneck for LARS is computing matrix-vector products. Therefore, a straightforward approach for parallelizing LARS is to make use of parallel matrix-vector products. There are numerous works on parallelizing matrix-vector product calculations [31]. In our experiments in Section 10 we do compare the two proposed methods with a LARS implementation that uses parallel matrix-vector products. Similarly, the proposed block LARS algorithm in Section 7 relies on matrix-matrix products which can also be efficiently parallelized [31]. The proposed tournament block LARS algorithm divides the problem into smaller problems that are solved in parallel and then we aggregate the results by allowing processors to compete. This strategy is similar to [13] for parallel QR and LU algorithms, where pivoting is performed in parallel by using a generalized tree reduction operation. Although we also use a generalized tree-reduction operation, at each leaf of the tree we perform a LARS operation and not a pivoting operation. Additionally, we modify a crucial part of the LARS algorithm, i.e., the calculation of the step-size, to guarantee that all steps are well-defined. Details are discussed in Section 8.

Recently, there have been numerous works regarding parallel optimization algorithms. $\ell_1$-regularization problems often appear in statistics [16], machine learning [28] and signal processing/compressed sensing [4] where there is a vast amount of data available, i.e., matrix $A$ has millions if not billions of samples and features. Large scale problems are the main reason for the resurgence in methods with computationally inexpensive iterations. Many modern first-order methods meet the previous goal. For instance, for $\ell_1$-regularized least-squares problems coordinate descent methods can have up to $n$ times less computational complexity per iteration than methods which use full gradient steps while at the same time it achieves very fast progress to optimality [27, 33, 41]. However, it is shown in [15] that the running time for such methods is often dominated by communication cost which increases with the number of processors. In the same work [15] the authors show how to avoid communication for an s-step accelerated proximal block coordinate descent and demonstrate up to 5x speedup compared to parallelized alternatives. Moreover, there are parallel accelerated and proximal coordinate descent methods [17] that do not use the s-step technique but allow coordinate updates to happen without synchronization. For example, HOGWILD! [32] is a lock-free approach to stochastic gradient descent (SGD) where each processor selects a data point, computes a gradient using its data point and updates the solution without synchronization. Finally, there are some frameworks and algorithms that attempt to reduce the communication bottleneck by reducing the number of iterations. For example, the CoCoA framework [21] reduces communication by performing coordinate descent on locally stored data points on each processor and intermittently communicating by summing or averaging the local solutions. Regarding $\ell_0$-regularization there are not many works in terms of parallel methods, a notable work is that of Needell and Woolf [26]. In this paper the authors suggest an asynchronous parallel and stochastic greedy algorithms, where multiple processors asynchronously update a vector in shared memory containing information on the estimated coefficients vector $\mathbf{x}$. Finally, one could also easily parallelize gradient-based methods for $\ell_1$ and $\ell_0$ regularization by parallelizing the computation of the gradients which relies in matrix-vector products.
Note that parallel optimization based methods aim in solving a single instance of $\ell_1$ or $\ell_0$ regularized least-squares, i.e., they produce a single sparse linear model. In this paper we are interested in algorithms that produce a sequence of sparse linear models.

5 Preliminaries and Assumptions

5.1 Preliminaries

Capital letters denote matrices, lower case bold letters denote vectors, lower case letters denote scalars and hollow letters denote sets. We denote with $0_n$ a vector of zeros of length $n$. Subscript $k$ denotes the $k$th iteration of the algorithm. The set of positive integers is denoted by $\mathbb{Z}_+$. We use $[::k]$ to denote a function with a vector as an input that returns a subvector which corresponds to the indices in the subscript set. $A^T$ denotes the transpose of a matrix. We denote with $A_{set}$ the concatenation of columns of matrix $A$ with indices in the subscript set. We denote the complement of a set by using the superscript $c$. We use the function $\text{sign}(\cdot)$ to denote the sign function which is applied component-wise if the input is a vector. We use the convention that $\text{sign}(0) = 0$. We define $\text{abs}(\cdot)$ as the absolute function which is often applied component-wise. We define the function $\text{max}^b(\cdot)$ and $\text{argmax}^b(\cdot)$ as the $b$th maximum of the input vector and the indices of the $b$ largest components of the input vector, respectively. If the input vector has less than $b$ components then the latter functions overwrite $b$ to be the length of the input vector. We define $\text{min}^-(\cdot)$ and $\text{argmin}^-(\cdot)$ similarly. The function $\text{min}^+(\cdot)$ returns the minimum positive value. The symbol $\emptyset$ denotes the empty set. We denote the simple multiplication of two scalars $a$ and $b$ by $a \cdot b$. By log we denote the logarithm with base 2.

5.2 Assumptions

For simplicity, we assume that the columns of matrix $A$ have unit $\ell_2$ norm, and that matrix $A$ is full-rank. For bLARS, we also assume that every $b$ columns are linearly independent. However, minor modifications to the algorithms can be done to bypass these assumptions. We assume that the communication cost includes the “bandwidth cost,” i.e., the number of words, sent among cores for synchronization purposes, and the “latency cost,” i.e., the number of messages sent.

6 Least angle regression

In this section we review the LARS algorithm. LARS is shown in Algorithm 1. The termination criterion in Step 2 of Algorithm 1 is arbitrary, one can choose other criteria such as a lower bound on the maximum absolute correlation $\|e_k\|_{\infty}$, see [16]. Let us explain the first iteration of the algorithm. Let us assume that at the 0th iteration we have response $y_0$, residual vector $r_0 = b - y_0$, correlation vector $c_0 := A^T r_0$ and maximum absolute correlation $c_0 := \max |c_0|$. The algorithm starts by choosing all columns that have maximum absolute correlation

$$I_0 := \{i \in [n] \mid |c_0[i]| = c_0\}. \tag{3}$$

The next decision step is how to set $I_1$ and $y_1$ using $I_0$ and $y_0$. We will define the update as $y_1 := y_0 + u_0 y_0$. This implies that we will have to define the vector $u_0$ and the step-size $\gamma_0$. Let us start with the definition of $u_0$. LARS defines $u_0$ as a unit-length vector that is equiangular with signed columns in matrix $A$ with index in $I_0$. It is easy to see that $u_0 := A_{I_0} (A_{I_0}^T A_{I_0})^{-1} \text{sign}(\{c_0[i] \mid i \in I_0\}) c_{00} h_0$, where $h_0 := ||A_{I_0} (A_{I_0}^T A_{I_0})^{-1} \text{sign}(\{c_0[i] \mid i \in I_0\}) c_{00}||^2_2$, satisfies the requirements. This means that $A_{I_0}^T u_0 = \text{sign}((c_0)_{I_0}) c_{00} h_0$, which in turn implies that subject to sign changes and because the columns of $A_{I_0}$ and $u_0$ are unit-length then $u_0$ is equiangular with all columns in $I_0$, with cosine $\pm c_{00} h_0$. To define $\gamma_0$ and to update $I_1$ based on $\gamma_0$ we will need first to understand how the update rule $y_1 := y_0 + u_0 y_0$ affects the correlation vector $c_1$ as a function of $\gamma_0$. For this we will make use of the auxiliary vector $a_0 := A^T r_0$ and we will use a different step-size $\gamma_j$ for each element $j$. In particular, we have that $[c_1]_j(\gamma_j) = A_j^T (b - y_0 - u_0 y_0) = [c_0]_j - [a_0]_j \gamma_j \forall j \in I_0$ and

$$[c_1]_j(\gamma_j) = \text{sign}((c_0)_j) (1 - \gamma_j h_0) c_0 \forall j \in I_0. \tag{4}$$

Equation (4) uses $[a_0]_{I_0} = A_{I_0}^T u_0 = \text{sign}(\{c_0[i] \mid i \in I_0\}) c_{00} h_0$ and that vector $[c_0]_{I_0}$ has components of magnitude equal to $c_0$ since it satisfies the definition in (3). Notice that if $\gamma_j = 1/h_0$ then $[c_1]_j(\gamma_j) = 0 \forall j \in I_0$, which means that the
least-squares problem is minimized with respect to the chosen columns in $\|_0$. Although tempting, this is not the goal of LARS since this is an aggressive strategy similar to Forward Selection. As we increase $\gamma_j$ from 0 to $1/h_0$ the absolute correlations in $\|_0$ are decreased identically, see (4). This is because the absolute correlations for the columns in $\|_0$ are equal. However, the absolute correlations in $\|_0$ might increase or decrease. LARS’ goal is to find a column in $\|_0$ whose absolute correlation becomes equal to the maximum absolute correlation as we increase $\gamma_0$. To find such a column we need to find $\gamma_j$ for each $j \in \|_0$ such that

$$c_0(1 - \gamma_j h_0) = \| [c_0]_j - \gamma_j [a_0]_j \|.$$

(5)

Such $\gamma_j$ will guarantee that column $j \in \|_0$ has the same absolute correlation as the columns with index in $\|_0$. It remains to check if (5) has a solution. It has two solutions, out of which we keep the minimum positive one

$$\gamma_j := \min + \left( \frac{c_0 - [c_0]_j}{c_0 h_0 - [a_0]_j}, \frac{c_0 + [c_0]_j}{c_0 h_0 + [a_0]_j} \right).$$

Out of all $\gamma_j$ where $j \in \|_0$ we choose the one with the minimum value $\gamma_0 := \min_{j \in \|_0^c} \gamma_j$. Note that the minimum step-size $\gamma_0$ corresponds to the column(s) in $\|_0$ that will be the first to have the same maximal absolute correlation as the columns in $\|_0$. Then LARS updates the set of selected columns as $\|_1 := \|_0 \cup \{ \arg \min_{j \in \|_0} \gamma_j \}$. The chosen column is the column with the least-angle which is where LARS gets its name from. Finally, having the step-size $\gamma_0$ we update the response $y_1 := y_0 + \gamma_0 a_0$.

It is easy to show that our claims above hold for any iteration $k$. Therefore, it is easy to show that LARS guarantees that $A_k \subset A_{k+1}$ and $|A_k| = |A_{k+1}| + 1 \forall k$. Moreover, LARS decreases the maximum absolute correlation $c_k$ until it finally is equal to zero for $k = \min(m,n)$. Furthermore, the columns in $A_k$ have maximum absolute correlations $\forall k$. Therefore using (4) we see that LARS decreases $\| c_k \|_\infty$ at each iteration, where $\| \cdot \|_\infty$ is the infinity norm, i.e., maximum absolute component of the input. Furthermore, note that LARS also decreases $\| c_k \|_{\infty,k} := \sum_k c_k$ of $k$ largest absolute components; as we will see later this is a property that bLARS generalizes but for the $k \cdot b$ largest components.

**Algorithm 1 LARS**

1: Initialize $k := 0$, $y_k := 0_n$, $r_k := b$, $c_k := A^T r_k$, $i := \arg \max |c_k|$, $c_k := \max |c_k|$, $\|_k := \{ i \}$, $t \leq \min(m,n)$
2: while $\|_k \leq t$ do
3: $u_k := A_{i_k}(A_{i_k}^T A_{i_k})^{-1} \text{sign}([c_k]_{i_k}) h_k c_k$, where $h_k := \| A_{i_k}(A_{i_k}^T A_{i_k})^{-1} \text{sign}([c_k]_{i_k}) c_k \|^{-1}$
4: $\gamma_j := \min + \left( \frac{c_j - [c_0]_j}{c_j h_0 - [a_0]_j}, \frac{c_j + [c_0]_j}{c_j h_0 + [a_0]_j} \right) \forall j \in \|_k$, where $a_0 := A^T u_k$
5: $y_k := \min_{j \in \|_k} \gamma_j$, $i := \arg \min_{j \in \|_k} \gamma_j$, $\|_{k+1} := \|_k \cup \{ i \}$
6: $y_{k+1} := y_k + u_i y_k$
7: $c_{k+1} := A^T r_{k+1}$, where $r_{k+1} := b - y_{k+1}$
8: $c_k := \max |c_k|$
9: $k := k + 1$
10: end while
11: Return $\|_k$, $y_k$

7 Parallel block Least Angle Regression

In this section, we describe one iteration of bLARS (without going into any details about parallelism), and then we explain how we can parallelize bLARS.

Let us assume that at the 0th iteration of bLARS we have response $y_0$, residual vector $r_0 = b - y_0$, correlation vector $c_0 := A^T r_0$ and the $b$th maximum correlation $c_0 := \max_b |c_0|$. The algorithm chooses all columns that have larger or equal absolute correlation than the maximum $b$th absolute correlation $\|_0 = \{ i \in [n] \mid \| [c_0]_i \| \geq c_0 \}$. Similarly to LARS, we define the update as $y_1 := y_0 + u_0 y_0$, but the decision rules for selecting $u_0$, $\gamma_0$ and updating $\|_0$ and $y_0$ are different. bLARS defines $u_0$ as $u_0 := A_{i_0}(A_{i_0}^T A_{i_0})^{-1} [c_0]_{i_0} h_0$ and $h_0 := \| A_{i_0}(A_{i_0}^T A_{i_0})^{-1} [c_0]_{i_0} \|^{-1}$. This means that $u_0$ is a unit-length vector that satisfies $A_{i_0}^T u_0 = [c_0]_{i_0} h_0$, instead of $A_{i_0}^T u_0 = \text{sign}([c_0]_{i_0}) c_0 h_0$ for LARS. Note that $u_0$ is not guaranteed to be equiangular to the chosen columns in $\|_0$. This is because $[c_0]_{i_0}$ is not guaranteed to have components with equal value. On the contrary, LARS guarantees that all components of
are equal to the maximum absolute correlation. However, bLARS still guarantees that there is no column that hasn’t been selected with absolute correlation larger than the bth maximum absolute correlation. Similarly to LARS, we will make use of the auxiliary vector \(a_0 := A^T u_0\), but we will use different step-sizes \(\gamma_j\) for each element \(j\). In particular, we have that \([c_1]_j(\gamma_j) = A^T_j (b - y_0 - u_0 \gamma_j) = [c_0]_j - [a_0]_j \gamma_j \forall j \in \mathbb{I}_0\), where \(\mathbb{I}_0\) is the complement of \(\mathbb{I}_0\), and

\[
[c_1]_j(\gamma_j) = [c_0]_j(1 - \gamma_j h_0) \forall j \in \mathbb{I}_0.
\]

The last equality uses \([a_0]_\mathbb{I}_0 = A^T \mathbb{I}_0 u_0 = [c_0]_\mathbb{I}_0 h_0\). This is different from LARS which uses \([a_0]_\mathbb{I}_0 = \text{sign}(\{c_0\}_\mathbb{I}_0) c_0 h_0\). This means that as we increase \(\gamma_j\), LARS decreases the absolute correlations identically, but bLARS decreases the absolute correlations with the same rate but not identically. However, bLARS still guarantees that if \(\gamma_j = 1/h_0\) then \([c_1]_j(\gamma_j) = 0 \forall j \in \mathbb{I}_0\), which means that the least-squares problem is minimized with respect to the chosen columns in \(\mathbb{I}_0\). Furthermore, bLARS still guarantees that as we increase \(\gamma_j\) from 0 to \(1/h_0\) the absolute correlations in \(\mathbb{I}_0\) are decreased, see (6), but the absolute correlations in \(\mathbb{I}_0\) might increase or decrease. bLARS goal is to find \(b\) columns in \(\mathbb{I}_0\) for which their absolute correlations become larger or equal to the minimum absolute correlation of columns in \(\mathbb{I}_0\) as we increase \(\gamma_j\). To find such a column we need to find \(\gamma_j\) for each \(j \in \mathbb{I}_0\) such that

\[
c_0(1 - \gamma_j h_k) = ||c_k - \gamma_j[a_k]||.
\]

Using the definition of \(c_0\), such \(\gamma_j\) will guarantee that column \(j \in \mathbb{I}_0\) has the same absolute correlation as the column with index \(i \in \mathbb{I}_0\) that satisfies \(i = \arg \max^b |c_0|\). Equation (7) has two solutions, we keep the minimum positive solution

\[
\gamma_j := \min^b \left( \frac{c_0 - [c_0]_j}{c_0 h_0 - [a_0]_j}, \frac{c_0 + [a_0]_j}{c_0 h_0 + [a_0]_j} \right).
\]

Out of all \(\gamma_j\) where \(j \in \mathbb{I}_0\) we choose the one with the minimum \(b\)th value \(\gamma_0 := \min^b \gamma_j\). Note that the \(b\)th minimum step-size \(\gamma_0\) corresponds to the column(s) in \(\mathbb{I}_0\) that will be the \(b\)th to have the same absolute correlation with the column in \(\mathbb{I}_0\) with the minimum absolute correlation. Then bLARS updates \(\mathbb{I}_j := \mathbb{I}_j \cup \{b\ \text{columns with } \gamma_j \geq \gamma_0\}\). Note that bLARS decreases \(||c_k||_{\infty, b} := \text{sum of } k \cdot b \text{ largest absolute components, compared to LARS which decreases } ||c_k||_{\infty}\). It is easy to see that by setting \(b = 1\) then bLARS is equivalent to LARS.

The parallel bLARS algorithm is shown in Algorithm 2. This algorithm is presented in great detail since this demonstrates our implementation. We assume that the data matrix \(A\) and any vector/set of length/cardinality \(m\) are partitioned across processors, i.e., each processor holds \(m/P\) components, where \(P\) is the number of processors and we assume for simplicity that \(m/P\) is an integer. More complicated two dimensional partitions could be used [5, 29], but we use row partition for simplicity. The main computational kernels of the algorithm are matrix-matrix and matrix-vector products, which we can parallelize efficiently using Message Passing Protocol (MPI) collective routines for reduction [36]. We also make use of collective routines for broadcasting data [36]. In our numerical experiments in Section 10, we use parallel bLARS with \(b = 1\) as parallel LARS.

### 7.1 Asymptotic costs for parallel bLARS and LARS

In what follows we examine the asymptotic costs of each step of parallel bLARS in Algorithm 2. The asymptotic costs of parallel LARS are obtained by setting \(b = 1\). We also comment when a step is executed only by the master processor, by all processors independently or in parallel with synchronization. We model the running time of an algorithm by considering both arithmetic and communication costs. In particular, we model the running time of an algorithm as a sum of three terms as

\[
\gamma F + \alpha L + \beta W,
\]

where \(\gamma\), \(\alpha\) and \(\beta\) are hardware parameters for time per arithmetic operation, time per message sent and time per word moved, respectively. \(F\), \(L\) and \(W\) are algorithm parameters for number of arithmetic operations to be executed, number of messages to be sent and number of words to be moved, respectively. We choose the \(\alpha-\beta\) model to measure communication of algorithms for simplicity. More refined models exists like the LogP [12] and LogGP [1] models.
Algorithm 2 Parallel bLARS for row-partitioned data

1: Initialize $b \in \mathbb{Z}_+, t \leq \min(m,n) \in \mathbb{Z}_+, k := 0, y_k := 0, r_k := b$ in parallel without synchronization.
2: Compute $c_k := A^T r_k$ in parallel using reduction.
3: $c_k := \max_i |c_k|, \Pi_k := \{i \in [n] \mid |c_k[i]| \geq c_k\}$.
4: Compute $G_k := A_k^T A_k$ in parallel using a reduction.
5: Compute $L_k$, the Cholesky factor of $G_k$
6: while $|\Pi_k| < t$ do
7: $s_k := [c_k]_{\Pi_k}, q_k := (L_k L_k^T)^{-1} s_k$
8: $h_k := (s_k q_k)^{-1}/2, w_k := q_k h_k$
9: The master processor broadcasts $w_k$.
10: Compute $u_k := A_k^T w_k$ in parallel, no communication is required.
11: Compute $a_k := A_k^T u_k$ in parallel using a reduction.
12: $\gamma_j := \min\left( \frac{c_{j-1}[i]-|c_j|}{c_{j-1}[i]+|c_j|}, \frac{c_{j+1}[i]-|c_j|}{c_{j+1}[i]+|c_j|} \right) \forall j \in \Pi_k$
13: $\gamma := \min_{j \in \Pi_k} \gamma_j$
14: $B := \arg \min_{j \in \Pi_k} \gamma_j$ (note this return $b$ indices)
15: $\Pi_{k+1} := \Pi_k \cup B$
16: The master processor broadcasts $\gamma_k$ to all processors.
17: Compute $y_{k+1} := y_k + u_k \gamma_k$ in parallel, no communication is required.
18: $[c_{k+1}] := [c_k](1 - \gamma_k h_k) \forall j \in \Pi_k$, and $[c_{k+1}] = [c_k] - \gamma_k [a_k] \forall j \in \Pi_k$
19: $c_{k+1} := c_k(1 - \gamma_k h_k)$
20: Compute $A_k^T A_B$ and $A_k^T A_B$ in parallel using a reduction.
21: $H_{k+1} := L_k^{-1} A_k^T A_B$
22: Solve $\Omega_{k+1} \Omega_{k+1} = A_k^T A_B - H_{k+1} H_{k+1}$ subject to $\Omega_{k+1}$ being a lower triangular matrix.
23: $L_{k+1} := \begin{bmatrix} L_k & 0_{0,b} \\ H_{k+1} & \Omega_{k+1} \end{bmatrix}$
24: $k := k + 1$
25: end while
26: Return $\Pi_k, y_k$

We assume that the data matrix $A$ and any vector/set of length/cardinality $m$ is partitioned across processors, i.e., each processor holds $m/P$ components, and $m/P$ rows of $A$, where $P$ is the number of processors and we assume for simplicity that $m/P$ is an integer. We also assume that matrix $A$ is a dense matrix. Step 1 requires $O(m/P)$ operations for initialization of $y_0$ and $r_0$ in parallel with no communication. Step 2 requires computing $c_k$ which is equal to $A^T r_k$. This operation can be performed in parallel with synchronization in $O(mn/P)$ operations, $n \log P$ words and $\log P$ messages, using a binary tree reduction algorithm in [36]. The result of Step 2 is reduced to the master processor. Step 3 is performed by the master processor and it costs $O(n \log n)$ operations using Heapsort, Section 5.2.3 in [23]. Step 4 is performed in parallel with synchronization and it requires $O(b^2 m/P)$ operations, $b^2 \log P$ words and $\log P$ messages using binary tree reduction. Step 5 is executed by the master processor and it costs $O(b^3)$ operations. Step 7 is executed by the master processor and it costs $O(|\Pi_k|)$ operations to compute $s_k := [c_k]_{\Pi_k}$. Since $|\Pi_k| = b(k+1)$, Step 7 costs $O(bk+b)$ operations. Moreover, Step 7 requires an additional $O(b^2 (k+1)^2)$ operations to compute $q_k := (L_k L_k^T)^{-1} s_k$, which is also executed by the master processor. Steps 8 costs $O(bk+b)$ operations and it is executed by the master processor. In Step 9 $w_k$ has to be broadcasted to each processor from the master processor and this costs $b(k+1) \log P$ words and $\log P$ messages using a broadcast algorithm from [36]. Step 10 is computed in parallel without synchronization in $O(b(k+1)m/P)$ operations, i.e., each processor multiplies its own part of the vector $A_k$ with $w_k$. Step 11 is executed in parallel with synchronization and it requires $O(mn/P)$ operations, $n \log P$ words and $\log P$ messages using a reduction. The result of Step 11 is reduced to the master processor. Step 12 is executed by the master processor and it requires $O(|\Pi_k|)$ operations, which is upper bounded by $O(n)$ operations in worst-case since $|\Pi_k| \leq n$. Steps 13 and 14 are executed by the master processor and they require in worst-case $O(n \log n)$ operations using Heapsort. Step 15 is executed by the master processor and it costs $O(b)$ operations. In Step 16 the step-size $\gamma$ is broadcasted to all processors from the master processor in $\log P$ words and $\log P$ messages. Step 17 is executed in parallel without synchronization and it requires $O(m/P)$ operations. Steps 18 and 19 are executed by the
master processor and they require $O(n)$ operations. Step 20 is executed in parallel with synchronization and it requires $O(b^2km/P + b^2m/P)$ operations, $O((b^2k \log P + b^2 \log P))$ words and $2 \log P$ messages. The result of Step 20 is reduced to the master processor. Step 21 is executed by the master processor and it requires $O((b^2k + b^2) \log P)$ operations since $L_k$ is a lower triangular matrix. Step 22 is executed by the master processor and it requires $O(b^2k + b^2)$ operations. Step 23 is executed by the master processor and it requires $O((b^2k + b^2) \log P)$ operations. Notice that if we want to obtain $t$ columns using LARS then we need to run the algorithm for $(t-1)/b$ iterations. Therefore, if we want to obtain $t$ columns using bLARS then we need to run the algorithm for $(t-1)/b$ iterations. By using this and the above costs for each step we summarize in Table 1 the asymptotic costs of bLARS and LARS for obtaining a solution with $t$ columns. Assuming that $t \gg b$, which means that we want to output many more columns than $b$, then we observe in Table 1 that by using bLARS we reduce by a factor of $b$ all major computational and communication costs compared to LARS.

### 8 Tournament block Least Angle Regression

In this section we will present tournament block LARS (Tournament-bLARS) a variation of LARS where $b$ columns are selected at each iteration using a generalized reduction on a binary tree. Like bLARS, Tournament-bLARS requires a lot of non-trivial modifications in order to maintain some properties of the original algorithm which we discuss in detail below. In comparison to parallel LARS and bLARS for Tournament-bLARS we assume that the data matrix $A$ is stored in a one-dimensional column partition, i.e., each processor holds $n/P$ rows, where $P$ is the number of processors and we assume that $n/P$ is an integer. Furthermore, we assume that vectors of length $m$ or $n$ or sets with cardinality at most $m$ or $n$ can be stored locally.

Let us now describe one iteration of T-bLARS. Let us assume that at the $l$th iteration we have response $y_l$ and we have selected columns $I_l$. Furthermore, let us assume that $P = 2$, i.e., 2 processors. Each processor gets $n/P$ columns, which we denote with index sets $I_{v_1}$ and $I_{v_2}$. T-bLARS requires running a modified version of LARS (mLARS), which we discuss later, as a reduction on a binary tree. For a visual explanation see Figure 1. The algorithm starts at the bottom of the tree by calling mLARS for each node in parallel. Nodes $v_1$ and $v_2$ return candidate columns with indices in the sets $B_{v_1}$ and $B_{v_2}$, respectively. Columns $B_{v_1} \cup B_{v_2}$ are sent to node $v_3$, which is the parent of $v_1$ and $v_2$. Finally, the node $v_3$ calls mLARS using columns in $I_l \cup B_{v_1} \cup B_{v_2}$ which returns the new response $y_{l+1}$ and index set $I_{l+1}$. Then this process is repeated. Details are provided in Algorithm 3.
Modified LARS. We mentioned that each node calls a modified version of LARS Algorithm 4. Let us now comment on this algorithm and why LARS needs to be modified in order for Tournament-bLARS to be a well-defined algorithm. The problem is caused due to the fact that each processor on any level of the binary tree runs mLARS independently of other processors and on data that might not overlap. This may result in violation of a basic rule of LARS, which is that there is no column that hasn’t been selected with larger absolute correlation than the current known maximum absolute correlation $c_k$.

Similarly to LARS, mLARS chooses one column at each iteration. Each call to mLARS operates on the columns with indices in $\mathbb{I}_v \cup \mathbb{I}_l$, where $v$ is the index of the node in the binary tree and $\mathbb{I}_l$ is the set of indices of columns that have been selected at the $l$th iteration of Tournament-bLARS. If $\mathbb{I}_l$ does not include any index with maximum absolute correlation among the indices in $\mathbb{I}_v \cup \mathbb{I}_l$, then equation (5) might not have a non-negative solution. This affects the step-size calculation, which for LARS is computed by solving equation (5) with the constraint that $\gamma \geq 0$. To guarantee that a meaningful step-size is calculated at each iteration of mLARS we propose using stepLARS in Procedure 1. Briefly, stepLARS detects violations to the above basic rule of LARS. If it detects a violation it checks if (5) still has a non-negative solution and sets $\gamma_k$ appropriately. If it cannot resolve it (equation 5 does not have a non-negative solution) then it sets $\gamma_k = 0$. By setting $\gamma_k = 0$ we guarantee that we do not update the response $y_k$ in current iteration. Setting $\gamma_k$ to a positive value would be a “mistake” since as we show in Step 14 of stepLARS Procedure 4 this would result in decreasing the current known maximum correlation $c_k$ of mLARS but at the same time it increases the absolute correlation of columns that violate the LARS property. This makes violation of the LARS property even larger.

If $\gamma_k = 0$ then mLARS at Step 18 adds the column with the largest absolute correlation that also violates the LARS property in the set of selected columns. This decision guarantees that a violation will not happen again during the execution of mLARS. This is because similarly to LARS, mLARS guarantees that once $c_k$ is maximal then it will remain like this for all iterations and this ensures that (5) always has at least one non-negative solution. More details are described in mLARS Algorithm 4 and Procedure 1.

8.1 Asymptotic costs for parallel implementation of Tournament-bLARS

In this subsection we examine the asymptotic costs for Tournament-bLARS Algorithm 3. We start first by the asymptotic costs of mLARS Algorithm 4, which is used by Tournament-bLARS at every iteration.

We assume that the data matrix $A$ is column-partitioned, i.e., each processor holds $n/P$ columns, where $P$ is the number of processors and we assume that $n/P$ is an integer. Furthermore, we assume that vectors of length $m$ or $n$ or sets with cardinality at most $m$ or $n$ can be stored locally.

Before we compute the asymptotic costs for mLARS we have to bound the cardinality of some sets. The cardinality $|\mathbb{I}_l|$ is bounded by $|\mathbb{I}_l| \leq n/P$. Let $l$ be the $l$th iteration of Tournament-bLARS, and $\mathbb{I}_l$ be the current selected columns of Tournament-bLARS. Then $|\mathbb{I}_l| \leq lb$. Assuming that we are on the $k$th iteration of mLARS then $|\mathbb{I}_k| \leq |\mathbb{I}| + b \leq lb + b$ and $|\mathbb{I}_k \cup \mathbb{I}_l \cup \mathbb{B}| \leq n/P + lb + b + 2b$ for all $k$. The cardinality of $\mathbb{I}_v \cup \mathbb{B} \setminus \mathbb{I}_k$ is bounded by $n/P + 2b$, since $|\mathbb{I}_v \cup \mathbb{B} \setminus \mathbb{I}_k| \leq |\mathbb{I}_v \cup \mathbb{B}| \leq n/P + 2b$. Using these bounds we will compute the asymptotic costs of each step of mLARS. Note that there is no parallelism for each individual run of mLARS. Therefore, we only report results for arithmetic operations.

Step 3 costs $O(m)$ operations. Step 4 costs $O(mn/P + mlb + 3mb)$. Step 5 costs $O(lb + b)$. Step 7 costs $O((n/P + lb + 3b) \log(n/P + lb + 3b))$. Step 10 costs $O(lb + b)$. Step 11 costs $O((lb + b)^2)$. Step 12 to 13 cost $O(lb + b)$. Step 14 costs $O(mlb + mb)$. Step 15 costs $O(mn/P + mlb + 3mb)$. Steps 16 to 18 cost $O((n/P + 2b) \log(n/P + 2b))$. Step 19 costs $O(m)$. Steps 20 to 21 cost $O(n/P + lb + 3b)$. Step 22 costs $O((lb + b) \log(lb + b))$. Step 23 costs $O(mlb + mb)$. Step 24 costs $O((lb + b)^2)$. Steps 25 to 26 cost $O(lb + b)$. For $t$ columns we need to run Tournament-bLARS for $t/b$ iterations and each iteration makes $\log P$ parallel calls to mLARS which results
Algorithm 3 T-bLARS

1: Initialize $l := 0$, $y_l := 0$, $t \in \mathbb{Z}_+$, $b \in \mathbb{Z}_+$, $L_l = 0$, where $L_l$ is the Cholesky factor.
2: Initialize $\mathbb{I}_l = \emptyset$
3: while $|\mathbb{I}_l| < t$ do
4:   for all levels of the tree from bottom to the root do
5:     if at the bottom of the tree then
6:        Let $\mathbb{B}_v$ be the columns of node $v$ in the tree. For all nodes $v$ in the current level of the binary tree call $B_v \leftarrow mLARS(b, y_l, I_l \cup \mathbb{B}_v, L_l)$.
7:     else if not at root of the binary tree then
8:        Let $\mathbb{B}_v$ be the columns selected by child nodes of $v$. For all nodes $v$ in the current level of the binary tree call $\tilde{B}_v \leftarrow mLARS(b, y_l, I_l \cup \mathbb{B}_v, L_l)$, where $\tilde{B}_v$ are the selected $b$ columns out of $\mathbb{B}_v$.
9:        Send columns $\tilde{B}_v$ for each node $v$ to the processor of the parent node of $v$.
10:    else
11:        $y_l+1, I_{l+1}, L_{l+1} \leftarrow mLARS(b, y_l, I_l \cup B_v, L_l)$
12:        Broadcast selected columns with index in $I_{l+1}$, $y_{l+1}$, and $L_{l+1}$ to all processors. Note that we only communicate the part of $L_{l+1}$ that gets updated by the root node.
13:   end if
14: end for
15: $l := l + 1$
16: end while
17: Return $I_l, y_l$

in $t/b \cdot (\text{arithmetic cost of mLARS}) \cdot \log P$ total operations. Therefore, in Big O notation Tournament-bLARS requires

$$F = O \left( \left( \frac{tmn}{bP} + \frac{t^2m}{b} + \frac{t^3}{b^2} \right) \log P \right)$$

operations. Communication occurs $\log P$ times because of the binary tree and another $\log P$ times to broadcast data from the root node to the rest of the nodes. Therefore Tournament-bLARS requires

$$L = 2t/b \log P$$

messages. Each node (except of the root) communicates $bm$ words for columns in $B$. Therefore the execution of the binary tree requires $bm \log P$ words. Broadcasting data from the root node to the rest of the nodes at Step 10 costs $(t^2m/b + tm + tm/b + t^2/b + tb) \log P$ words. By assuming that $t \gg b$ and using Big O notation we have a total of

$$W = O \left( \left( \frac{t^2m}{b} + tb \right) \log P \right)$$

words.

9 Comparison of asymptotic costs

In this section, we compare the asymptotic costs of parallel LARS, bLARS and T-bLARS. The results are shown in Table 2. Note that parallel bLARS becomes faster than parallel LARS for $b > 1$. The comparison between T-bLARS and LARS is not so clear. However, it is easy to see that as $b$ and $P$ increase then T-bLARS could be faster depending on the hardware parameters. We extensively investigate this comparison by empirical observations in Section 10. Parallel bLARS and T-bLARS have similar arithmetic and latency costs. However, an important difference is that the number of words for parallel bLARS depends on the number of columns $n$ while the number of words for T-bLARS depend on the number of rows $m$. This is due to the fact that for parallel bLARS we partition the data per row, while for T-bLARS we partition the data per column. We compare the two methods empirically in Section 10.
We present a comprehensive list of plots extracted from the regression datasets summarized in Table 3. We use working with are large, we limit the algorithm to only collect the first 50 columns. For our implementation, we have used a Python implementation of the code and the optimized mpi4py library. We used a shared memory that display the performance gains with regards to thread count (P) and block size (tmn).

10 Empirical performance

We present a comprehensive list of plots extracted from the regression datasets summarized in Table 3. We use two metrics to measure performance. One metric is, for a given parameter b, the value of the ℓ₂-norm of the residual vector versus the number of columns added at each iteration (Figure 3). We also consider speed-up from increasing the block size b and thread count P (Figure 2). Regarding the speed-up metric, we present heatmaps that display the performance gains with regards to thread count (P) and block size (b). Since the datasets we are working with are large, we limit the algorithm to only collect the first 50 columns. For our implementation, we have used a Python implementation of the code and the optimized mpi4py library. We used a shared memory computer with Intel 2x Intel E5-2670 (8C), 128 GB of RAM.

In Figure 2, we show the speed-up trends for YearPredictionMSD, E2006 and sector datasets, respectively, from left to right (top is bLARS, bottom is T-bLARS). We can make performance insights depending on the matrix shape. For tall, row-partitioned matrices like YearPredictionMSD, we see how increasing the thread count and block count results in improved performance. We get good speed-ups (up to 25x) in bLARS. However, we

| Method       | Arithmetic operations | Words communicated | Messages |
|--------------|-----------------------|--------------------|----------|
| LARS         | \(\frac{tmn}{P} + tn \log n + \frac{t^2m}{P} + t^3\) | \(tn \log P + t^2 \log P\) | \(t \log P\) |
| bLARS        | \(\frac{tmn}{bP} + \frac{tn \log n}{b} + \frac{t^2m}{P} + t^3\) | \(\frac{tn}{b} \log P + t^2 \log P\) | \(\frac{t}{b} \log P\) |
| T-bLARS      | \(\left(\frac{tmn}{bP} + \frac{t^2m}{bP} + \frac{t^3}{b}\right) \log P\) | \(\left(\frac{t^2m}{b} + tb\right) \log P\) | \(\frac{t}{b} \log P\) |

Table 2: Asymptotic costs for parallel LARS, bLARS, T-bLARS. Here, \(t\) is the required number of columns to be outputted by all algorithms. We assume that \(t \gg b\) and that matrix \(A\) is dense.
Algorithm 4 Modified Least Angle Regression (mLARS)

1: Input: number of columns $b \in \mathbb{Z}_+$, response $\mathbf{y}$, $\mathbf{1}$ (third input), column index sets $\mathcal{I}_v$ (third input) and Cholesky factor $L$ (forth input)
2: Initialize: $k := 0$, $\mathcal{B} := \emptyset$, $L_k := L$, $\mathcal{I}_k := \mathcal{I}$
3: $\mathbf{r}_k := \mathbf{b} - \mathbf{y}$
4: $\mathbf{c}_k := \mathbf{A}^T_{\mathcal{I}_k \cup \mathcal{B}} \mathbf{r}_k$
5: $c_k := \max ||\mathbf{c}_k||_2$. Note that we abuse notation here for $[\mathbf{c}_k]_{I_k}$. Since $\mathbf{c}_k \in \mathbb{R}^{||\mathcal{I}_k \cup \mathcal{B}||}$ and by usual convention its components are indexed from 1 to $||\mathcal{I}_k \cup \mathcal{I}_v \cup \mathcal{B}||$ which might not overlap with the indices in $\mathcal{I}_k$. We assume that the components of $\mathbf{c}_k$ are indexed using the indices in $\mathcal{I}_k \cup \mathcal{I}_v \cup \mathcal{B}$. We use this abuse of notation at other steps of this algorithm because it simplifies notation.
6: if $\mathcal{I}_k = \emptyset$ then
7: $c_k := \max ||\mathbf{c}_k||$, $\mathcal{I}_k := \{ \arg \max ||\mathbf{c}_k|| \}$, $L_k = (A^T_{\mathcal{I}_k} A_{\mathcal{I}_k})^{1/2}$.
8: end if
9: while $|\mathcal{I}_k| < |\mathcal{I}| + b$ do
10: $\mathbf{s}_k := [\mathbf{c}_k]_{I_k}$
11: $\mathbf{q}_k := (L_k L_k^T)^{-1} \mathbf{s}_k$
12: $h_k := (\mathbf{s}_k^T \mathbf{q}_k)^{-1/2}$
13: $\mathbf{w}_k := \mathbf{q}_k h_k$
14: $\mathbf{u}_k := A^T_{\mathcal{I}_k} \mathbf{w}_k$
15: $\mathbf{a}_k := A^T_{I_k \cup \mathcal{B}} \mathbf{u}_k$
16: $\gamma_j \leftarrow \text{stepLARS}(c_k, h_k, \mathbf{a}_k, j) \forall j \in \mathcal{I}_v \cup \mathcal{B} \setminus \mathcal{I}_k$
17: If there are $\gamma_j$ that are equal to zero, set $\gamma_j$ to zero. Otherwise, set $\gamma_k$ to the minimum nonzero $\gamma_j$.
18: If there are $\gamma_j$ that are equal to zero, set $i$ to the $j$th column with the largest $||[\mathbf{c}_k]_j||$. Otherwise, set $i$ to the $j$th column with the minimum nonzero $\gamma_j$.
19: $y_{k+1} := y_k + u_i \gamma_k$
20: $[\mathbf{c}_{k+1}]_j := [\mathbf{c}_k]_j (1 - \gamma h_k) \forall j \in \mathcal{I}_k$, and $[\mathbf{c}_{k+1}]_j := [\mathbf{c}_k]_j - \gamma \mathbf{a}_k \mathbf{e}_j \forall j \in \mathcal{I}_v \cup \mathcal{B} \setminus \mathcal{I}_k$
21: $\mathcal{I}_{k+1} := \mathcal{I}_k \cup \{i\}$, $\mathcal{B} := \mathcal{B} \cup \{i\}$
22: $c_{k+1} := \max ||[\mathbf{c}_{k+1}]_{\mathcal{I}_{k+1}}||$
23: Compute $A^T_{\mathcal{I}_k} A_I$ and $A^T_I A_I$.
24: $L_{k+1} := L_k A^T_{\mathcal{I}_k} A_I$
25: $\omega_{k+1} := (A^T_{\mathcal{I}_k} A_I - I_{\mathcal{I}_{k+1}})^{1/2}$
26: $L_{k+1} := \left[ \begin{array}{c} L_k \\ 0_k \\ \omega_{k+1} \end{array} \right]$
27: $k := k + 1$
28: end while
29: Return $\mathbf{y}_k$, $\mathcal{I}_k$, $\mathcal{B}$, $L_k$

| Dataset              | $m$  | $n$  | nnz($A$)/$mn$ |
|----------------------|------|------|---------------|
| YearPredictionMSD    | 463715 | 90   | 1.00          |
| E2006_tfidf          | 16087 | 150360 | 0.008        |
| sector               | 6412  | 55197 | 0.003        |

Table 3: Properties of the data sets that we consider. nnz($A$) denotes the number of nonzeros in matrix $A$, consequently, the fourth column gives the (relative) sparsity of $A$. The regression datasets can be downloaded from [7] as part of the LIBSVM Data package.

do not observe the same speed-up for T-bLARS. In fact, we observe a slowdown for T-bLARS. On the other hand, T-bLARS is efficient for wide, column-partitioned matrices like in the sector and E2006 datasets. Based on Figure 2, it might seem that bLARS is still the better choice because of the large speed-ups it can accomplish as opposed to T-bLARS. However, it is important to note that the performance of bLARS in this case does not scale at all as we increase the thread count. T-bLARS, however, gets steady speed-ups from not only increasing the block size, but also the thread count. This indicates that T-bLARS is generally more well-suited to exploit the
In Figures 4 and 5 we present speed-up results for bLARS and T-bLARS when 25 and 75 columns are chosen, respectively. Similar trends are observed as in our discussion in the main paper where 50 columns are chosen in our experiments. Note that bLARS achieves very large speedup as \( b = 2 \) for bLARS, while for T-bLARS all settings achieved similar residual. If our objective is to achieve low residual for all iterations, then T-bLARS obtains 4x speed-up (\( P = 8, b = 26 \)) or (\( P = 8, b = 32 \)), while bLARS obtains 2x speed-up (\( b = 2 \)). In short, T-bLARS can accomplish better or similar speed-up of higher solution quality.

In Figures 2 and 6(b) we see that for the E2006 dataset the setting that achieves residual similar to LARS is \( b = 2 \) for bLARS, while for T-bLARS all settings achieved similar residual. If our objective is to achieve low residual for all iterations, then T-bLARS obtains 4x speed-up (\( P = 8, b = 26 \)) or (\( P = 8, b = 32 \)), while bLARS obtains 2x speed-up (\( b = 2 \)). In short, T-bLARS can accomplish better or similar speed-up of higher solution quality.

The two parallel and communication-avoiding methods we have introduced, bLARS and T-bLARS, present valuable methods of least-angle regression that provide higher performance of speed than LARS can normally give. The choice between the two comes down to understanding which matrices favor which method (row-partitioned for bLARS, column-partitioned for T-bLARS) and what priorities and expectations the user has from the solutions generated from these algorithms, e.g., be it higher speed or more resilient accuracy.

11 Conclusions
Figure 3: Solution quality plots. For T-bLARS each line corresponds to a setting of $P$ and $b$. We do not show all legends for T-bLARS to ease readability, most settings give similar quality. For bLARS each line corresponds to a different $b$. Note that $P$ does not affect the quality of bLARS.

Figure 4: Speed-up results vs. LARS. 25 columns where chosen for all experiments. The numbers inside the box demonstrate speed-up.
Figure 5: Speed-up results vs. LARS. 75 columns where chosen for all experiments. The numbers inside the box demonstrate speed-up.

Figure 6: Solution quality plots. For T-bLARS each line corresponds to a setting of $P$ and $b$. We do not show all legends for T-bLARS to ease readability, most settings give similar quality. For bLARS each line corresponds to a different $b$. Note that $P$ does not affect the quality of bLARS.
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