

MapReduce TSQR: using Apache Hadoop for Large-scale QR Decompositions of Tall and Skinny Matrices

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1 Motivation

The QR decomposition is one of the most common matrix decompositions in scientific computing. QR is one of the most common methods for solving least squares problems [9]. In many situations, we get overdetermined problems, i.e., when the number of rows is larger than the number of columns. We refer to these matrices as tall and skinny (TS) and thus we have tall and skinny QR decompositions. In this project, we look at two TSQR algorithms, one that uses the TSQR algorithm by Demmel et al. [8] and one that uses Cholesky QR. See sections 2 and 3.

With current trends towards “large data”, we face a challenge in scaling our software to handle more information. MapReduce is a programming model for application developers to scale code. Apache Hadoop [11] is a software framework for running MapReduce programs. Companies like Google, Facebook, IBM, and Microsoft have adopted these frameworks [12]. A major reason for the adoption of Hadoop and similar software is reliability: failed nodes in the cluster do not result in a failed job. We investigate the relationship between performance and faults in section 9.

In this project, we use Hadoop for computing QR decompositions using NERSC’s Magellan cloud testbed [14]. The ideas and code for this project are derived from similar work by Constantine and Gleich [6] [10]. We investigate large matrices on the order of 500 GB in size, which necessitates a cluster, rather than a single computer. Sections 4, 5, and 6 discuss implementation. Sections 6, 7, and 9 detail performance results. Lastly, section 8 looks at numerical stability.

2 TSQR

The $A = QR$ factorization factors an m by n matrix A into an m by n orthogonal matrix Q and an n by n upper triangular matrix R . Let A be a $4n$ by n matrix. We formulate a simple case of the TSQR algorithm as follows [8]:

$$A = \begin{pmatrix} A_1 \\ A_2 \\ A_3 \\ A_4 \end{pmatrix} = \begin{pmatrix} Q_1 R_1 \\ Q_2 R_2 \\ Q_3 R_3 \\ Q_4 R_4 \end{pmatrix} \rightarrow \begin{pmatrix} R_1 \\ R_2 \\ R_3 \\ R_4 \end{pmatrix} = \begin{pmatrix} Q_5 R_5 \\ Q_6 R_6 \end{pmatrix} \rightarrow \begin{pmatrix} R_5 \\ R_6 \end{pmatrix} = Q_7 R_7. \quad (1)$$

Each intermediate $Q_i R_i$ factorization is a local factorization. A_i and Q_i are n by n for $i = 1, 2, 3, 4$, Q_i is $2n$ by n for $i = 5, 6$ and Q_7 is $4n$ by n . R_i is n by n for $i = 1, 2, \dots, 7$. The QR decomposition is given by $A = QR_7$, where Q is constructed from the Q_i by equation 2:

$$Q = \begin{pmatrix} Q_1 & & & \\ & Q_2 & & \\ & & Q_3 & \\ & & & Q_4 \end{pmatrix} \begin{pmatrix} Q_5 & \\ & Q_6 \end{pmatrix} Q_7 \quad (2)$$

The horizontal lines in equation 1 represent opportunities for parallelism. The intermediate $Q_i R_i$ factorizations can be done in parallel at each step. This leads to a natural *logp* reduction, where A is split into A_1, \dots, A_p .

3 Cholesky QR

The $A = LL^T$ Cholesky factorization factors a symmetric positive definite matrix A into a lower triangular matrix multiplied by its transpose. We use the QR factorization to solve the normal equations:

$$x = (A^T A)^{-1} A^T b = (R^T Q^T Q R)^{-1} R^T Q^T b = (R^T R)^{-1} R^T Q^T b = R R^{-T} R^T Q^T b = R^{-1} Q^T b \quad (3)$$

Equation 3 leads to a back solve of $Rx = Q^T b$.

To solve the least squares problem with Cholesky, we note that $A^T A$ is symmetric and assume $A^T A$ is positive definite and write:

$$x = (A^T A)^{-1} A^T b = (LL^T)^{-1} A^T b \rightarrow LL^T x = A^T b \quad (4)$$

Equation 4 leads to a forward solve $L(L^T x) = Ly = A^T b$ and then a back solve $L^T x = y$. In exact arithmetic, Cholesky QR gives us the same information as TSQR. However, computing $A^T A$ squares the condition number of the problem, so Cholesky QR is less stable. We will investigate the trade-offs in section 7. A second way of interpreting R via Cholesky is given in equation 5.

$$A^T A = (QR)^T QR = R^T Q^T QR = R^T R = LL^T \quad (5)$$

4 Applying the MapReduce model to QR

In general, the Map Reduce model follows an iterative three-step process using key-value pairs. Let k_i and v_i represent keys and values, respectively, for $i = 1, 2, 3$. Then we can represent the three-step process by the composition of three functions:

$$(k_1, v_1) \xrightarrow{\text{map}} (k_2, v_2) \xrightarrow{\text{combine}} (k_2, v_2) \xrightarrow{\text{reduce}} (k_3, v_3)$$

For simplicity, we will ignore the combine step and only consider the map and reduce steps:

$$(k_1, v_1) \xrightarrow{\text{map}} (k_2, v_2) \xrightarrow{\text{reduce}} (k_3, v_3)$$

v_2 is treated as a list of values emitted by the map function all corresponding to a given key. We will use the following notation to indicate how many map and reduce tasks are used in a given iteration:

$$(k_1, v_1) \xrightarrow[nm]{\text{map}} (k_2, v_2) \xrightarrow[nr]{\text{reduce}} (k_3, v_3) \quad (6)$$

Equation 6 indicates that there are nm map tasks and nr reduce tasks. We will let max indicate that the maximum available tasks will be used.

We will denote the MapReduce model for TSQR and Cholesky QR by MRTSQR and MRCQR, respectively.

4.1 MRTSQR

The parallelism for TSQR is evident in the parallel local QR decompositions in section 2. MRTSQR uses both the map and reduce steps to perform local QR decompositions on leftover intermediate R_i . The functions look like:

$$(k, A_i) \xrightarrow{QR} (k, R_i) \xrightarrow{QR} (k, R_i).$$

Each map and reduce task outputs one intermediate R_i . In order to combine the results from the distributed reduce tasks, we introduce a second iteration:

$$(k, A_i) \xrightarrow[1]{QR} (k, R_i) \xrightarrow[1]{QR} (k, R_i) \xrightarrow[1]{identity} (k, R_i) \xrightarrow[1]{QR} (i, R). \quad (7)$$

A visual interpretation of equation 7 is given in Figure 1.

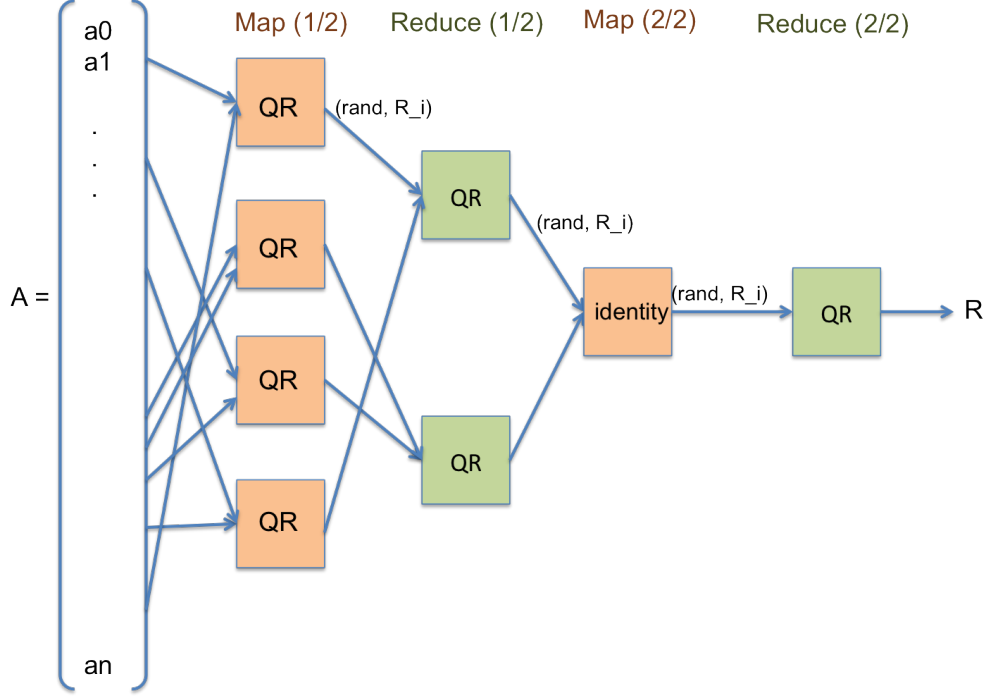


Figure 1: MRTSQR scheme

4.2 MRCQR

The MapReduce model for Cholesky QR is achieved by the parallelism in computing $A^T A$. A block of rows of A forms a matrix B , and $B^T B$ is computed locally. Then, the local $B^T B$ matrices are summed together. To sum the local $B^T B$, we keep track of the row numbers and have the reducers perform a row sum, as shown in equation 8.

$$(k, A_i) \xrightarrow[\max]{A^T A} (i, (A^T A)_i) \xrightarrow[\min(\max, n)]{\text{rowsum}} (i, (A^T A)_i) \xrightarrow[\min(\max, n)]{\text{identity}} (i, (A^T A)_i) \xrightarrow[1]{\text{Cholesky}} (i, R_i) \quad (8)$$

Theoretically, we expect a *logp* reduction tree on the row sums to get the best performance. However, the Hadoop overhead at each iteration makes this less appealing (see section 7.2). We get a local $A^T A$ from each map tasks, so we only need to perform $\#(\text{maptasks})$ vector sums per row. In our working examples, $\#(\text{maptasks})$ is at most a few thousand.

Unlike MRTSQR, we have steps with non-trivial keys. The row sum reducers must combine all records corresponding to a given row. The number of tasks in our first reduction step and second map step is limited by the number of keys for $A^T A$. If A is m by n , then $A^T A$ is n by n , so we can only use at most n tasks as the keys are given by the row number of $A^T A$.

A visual interpretation of the MRCQR job is given in Figure 2.

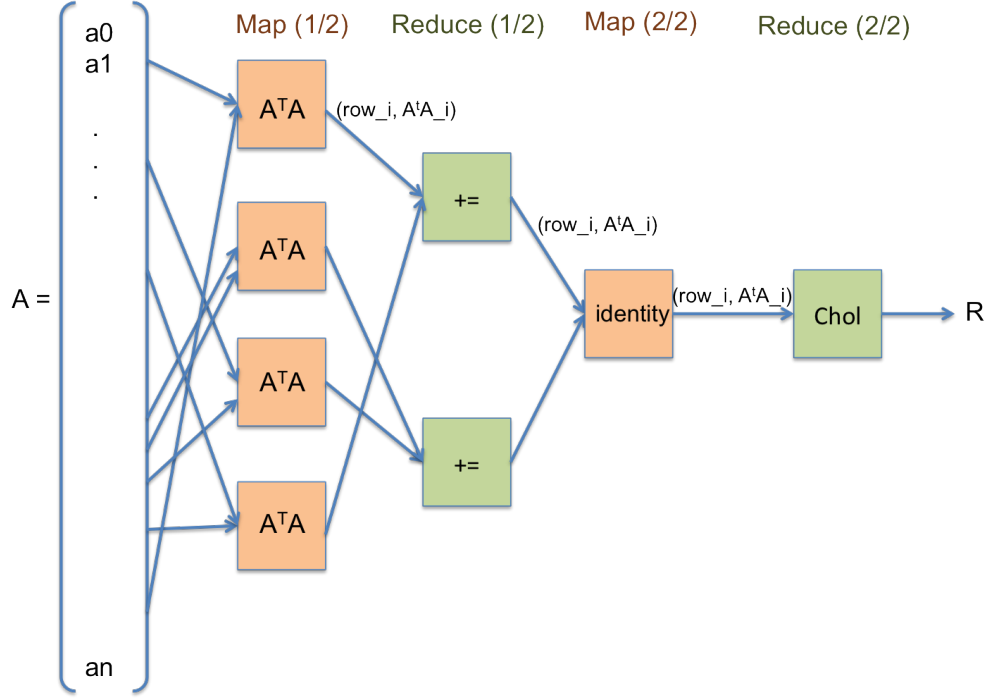


Figure 2: MRCQR scheme

5 Tools

5.1 Software

We employ a number of software tools. They are listed here with references for more information.

1. Apache Hadoop version 0.20.2 [11]
2. NumPy, a Python math library [15]
3. Dumbo, a Python framework for running Hadoop jobs (publicly available at [4])
4. Python TypedBytes support (publicly available at [3])
5. MRTSQR and MRCQR code (publicly available at [2] and [10])

5.1.1 Why so much Python?

Typically, high-performance computing employs lower-level languages like C/C++. In this project, Python was used extensively for several reasons. First, prototyping MapReduce schemes is much easier. Full implementations of the MRTSQR and MRCQR codes fit in around 100 lines of code. See Figure 5.1.1, which gives the entire Cholesky MRTSQR code in 58 lines of code. Second, NumPy provides interfaces to BLAS, so the computation time does not differ that much (see section 7.1). An investigation of the performance of C++ implementations against Python implementations for Hadoop streaming is in section 7.1.

5.2 Hardware

All experiments in the project were run on the Magellan cluster [14] at the National Energy Research Scientific Computing Center (NERSC). Magellan consists of an 80-node Hadoop cluster. Each node has two quad-core Intel Nehalem 2.67 GHz processors and a 1 TB (local) SATA disk. The network topology consists of local fat-trees with a global 2D mesh with InfiniBand fibre optic cables. The Hadoop cluster dedicates 6 cores/node to map tasks and 2 cores/node to reduce tasks. The theoretical peak performance of a node is about 85 GFlops [7]. Thus, the theoretical peak of the system is $80 \times 85 = 6800$ GFlops. We investigate peak performance more in section 7.3.

6 Data serialization optimizations

6.1 Techniques

6.1.1 TypedBytes storage formats

In a MapReduce architecture, we generally compute on large amounts of data. Thus, it is important to maintain the communication-avoiding algorithmic paradigm in order to keep our algorithms fast. In the Hadoop Distributed File System (HDFS), data is stored as a sequence of records, where each record is a key-value pair. Hadoop MapReduce jobs use an `InputFormat` class to validate and split up data and a `RecordReader` class to extract the key-value pairs.

Hadoop allows for user-defined input formats and record readers. In this project, Hadoop’s `AutoInputFormat` was used, which differentiates between text and sequence files and parses them accordingly. Typically, sequence files were used, which have better performance. The keys and values in a sequence file are stored as `TypedBytes`, and this storage format can store a variety of data types:

```
import random, struct, numpy, dumbo
class Cholesky(dumbo.backends.common.MapRedBase):
    def __init__(self,ncols):
        self.data = range(ncols)
        self.ncols = ncols

    def __call__(self,data):
        for key,values in data:
            for value in values:
                self.data[key] = list(struct.unpack('d'*self.ncols, value))

        for ind, row in enumerate(numpy.linalg.cholesky(self.data)):
            yield ind, row

class AtA(dumbo.backends.common.MapRedBase):
    def __init__(self,blocksize,isreducer,ncols):
        self.blocksize=blocksize
        self.isreducer=isreducer
        self.data = []
        self.ncols = ncols
        self.A_curr = self.row = None

    def compress(self):
        A_flush = numpy.mat(self.data).T*numpy.mat(self.data)
        self.data = []
        if self.A_curr == None:
            self.A_curr = A_flush
        else:
            self.A_curr = self.A_curr + A_flush

    def collect(self,key,value):
        self.data.append(value)
        if len(self.data)>self.blocksize*self.ncols:
            self.compress()

    def close(self):
        self.compress()
        for ind, row in enumerate(self.A_curr.getA()):
            r = [float(v) for v in row]
            yield ind, struct.pack('d'*len(r),*r)

    def __call__(self,data):
        if self.isreducer == False:
            for key,value in data:
                self.collect(key, list(struct.unpack('d'*self.ncols, value)))
        else:
            for key,values in data:
                for value in values:
                    val = list(struct.unpack('d'*self.ncols, value))
                    if self.row == None:
                        self.row = numpy.array(val)
                    else:
                        self.row = self.row + numpy.array(val)
                    yield key, struct.pack('d'*len(self.row),*self.row)

        if self.isreducer == False:
            for key,val in self.close():
                yield key, val
```

Figure 3: Full python MRCQR implementation (58 lines of code, including white space)

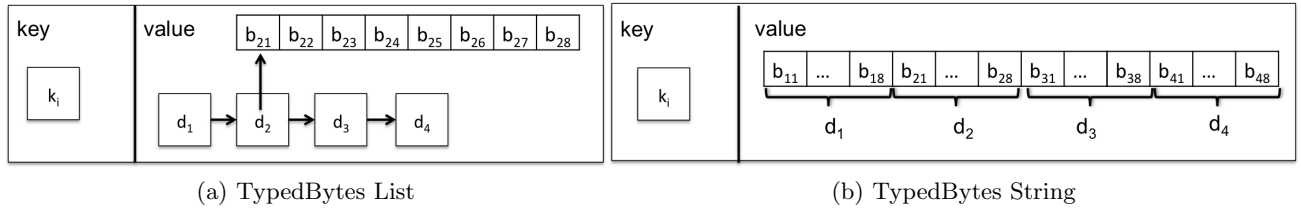


Figure 4: Simplified models of `TypedBytes` data structures

- Fixed-length data types: Byte, Bool, Int, Long, Float, Double
- Variable-length data types: Bytes, String, Vector, List

In this project, we evaluated performance differences from these data types. The original implementation by Constantine and Gleich [6] uses a `TypedBytes List` format, which maintains the list structure in the record. In order to reduce the amount of metadata moved by Hadoop jobs, a `TypedBytes String` format was used. The python `struct` module allows for reading and writing this data type (see [2], [10] for implementation details). Figure 4 illustrates the difference between a `TypedBytes List` and `TypedBytes String`. See section 6.2 for performance results.

6.1.2 Row packing

The second type of data serialization used is row packing. Typically, we store the matrix with one row per record. For very skinny matrices, it can be beneficial to store multiple rows in one record. For the experiments in section 6.2, we look at matrices with 4, 10, and 200 rows.

6.2 Experiments and Performance

Experiments were performed on three different matrices: (1) 20 billion by 4 (~ 600 GB), (2) 800 million by 10 (~ 60 GB), (3) 200 million by 200 (~ 300 GB). Tests were performed 5 times, represented by the x-axis as trials in Figures 5, 6, and 7. We expect that each matrix will benefit from the `TypedBytes String` format. We also expect that matrices with a smaller number of columns will benefit more from packed rows. These experiments were performed with the MRTSQR algorithm.

All three matrices benefited extraordinarily from the switch from a `TypedBytes List` to a `TypedBytes String` storage format. Speedups from this optimization were approximately 1.7-2x. Packed rows also resulted in significant speedups. With the 20 billion by 4 matrix, packing two rows per record resulted in an additional 20% performance increase, and packing four rows per record resulted in another additional 20%. With the 800 million by 10 matrix, we see that packing two row per record increased performance, but packing four rows per record resulted in erratic performance. With the 200 million by 2 matrix, packing two rows per record left the performance approximately unchanged.

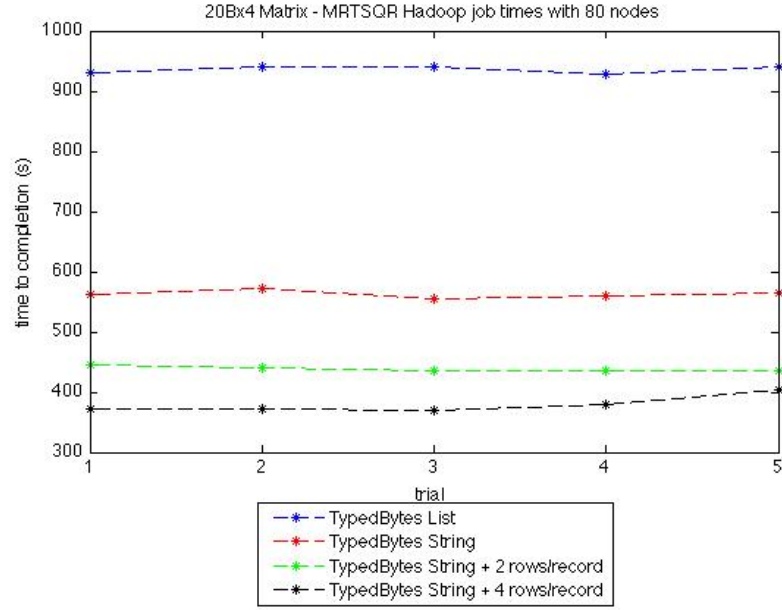


Figure 5: Performance of 20,000,000,000 x 4 matrix over a number of trials

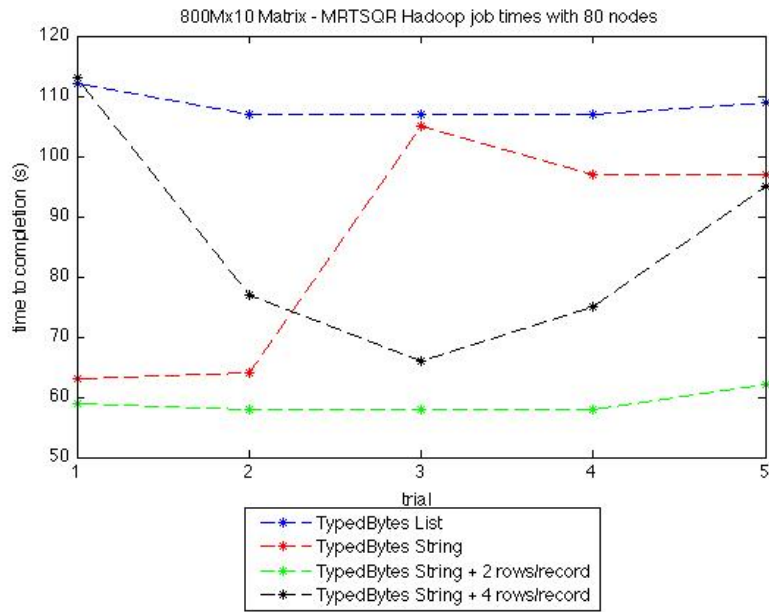


Figure 6: Performance of 800,000,000 x 10 matrix over a number of trials

Another important characteristic of the performance of the TypedBytes String storage format

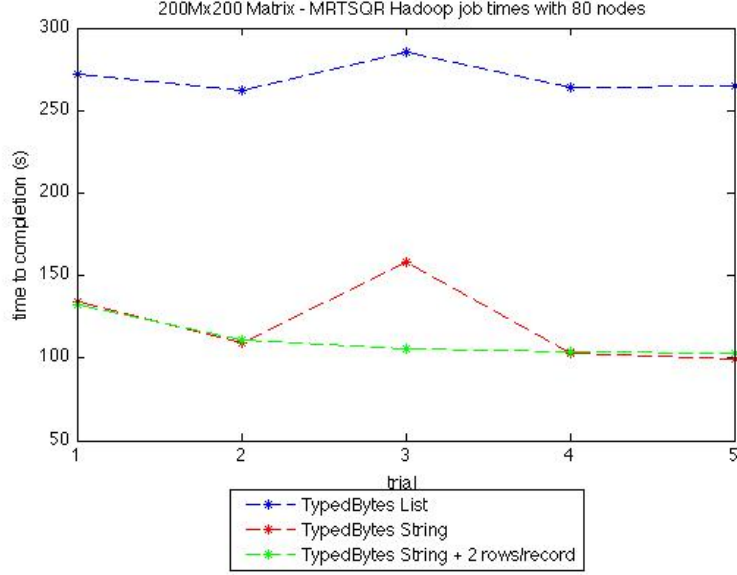


Figure 7: Performance of 200,000,000 x 200 matrix over a number of trials

and the packed rows is the amount of time spent generating the matrices. In these experiments, the matrices are synthetic. However, in applications, matrix storage and data processing could be two separate stages of the data analysis process. Because of this, it is important to recognize how long it takes to write out these matrices to disk. Figure 8 shows how long it took to generate the 800 million by 10 and 200 million by 200 matrices. We see that for the 800 million by 10 matrix, the TypedBytes String format and the row packing have significant affects on the matrix generation time. For the 200 million by 200 matrix, the TypedBytes String format produces 2.25x speedups in write times. However, row packing does not help with the generation time of this matrix.

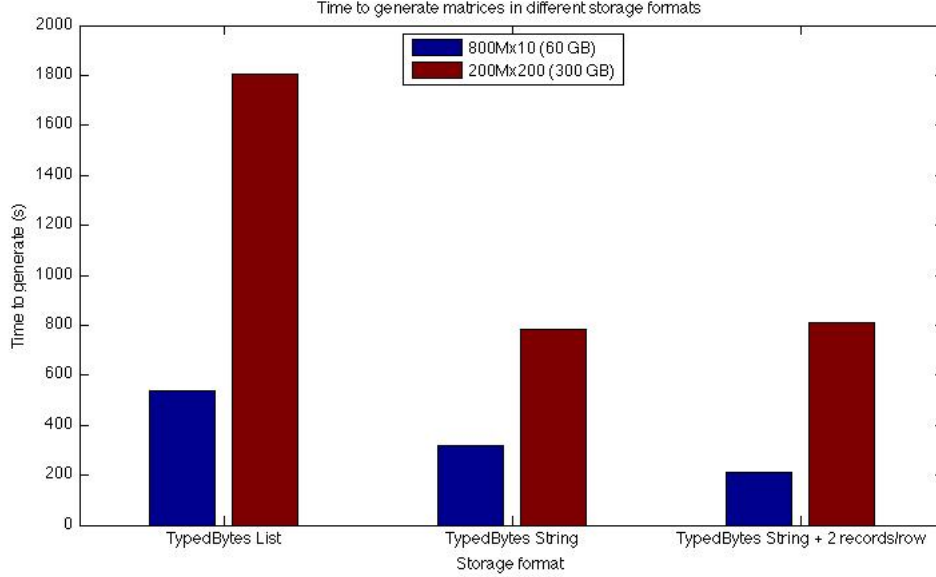


Figure 8: Time to generate the 800,000,000 x 10 and 200,000,000 x 200 matrices

7 Performance

7.1 Benchmarking MRTSQR and MRCQR for Python and C++

Figures 9 and 10 benchmark the Python implementations of the Cholesky QR and TSQR algorithms for two different matrices over a number of trials. The graphs also show the average amount of time spent in NumPy per core. In these experiments, there were 78 nodes, which in total gives $78 \times 8 = 624$ cores. The average NumPy time per core was calculated using a global Hadoop counter, where each Hadoop task increments the counter for each computation. This total time is then divided by 624.

Figure 9 shows the results for a 200 million by 200 matrix. For this matrix, Cholesky QR is about 10% faster than TSQR. Also, Cholesky QR spends about half the time doing computation. It is also worth noting that the time spent performing computation is much smaller than the total running time.

Figure 10 shows the results for a 800 million by 10 matrix, and the results are different. The difference between the Cholesky QR and TSQR algorithms is less pronounced, and the average NumPy time per core is negligibly small for both algorithms. This makes sense because the local factorizations have 10 columns instead of 200, so we expect communication to dominate overall running time even more.

Figures 11 and 12 benchmark the C++ implementations of the Cholesky QR and TSQR algorithms. Figure 11 shows the total running time for the two algorithms on two different matrices (800 million by 10 and 20 billion by 4) with packed rows. The TSQR algorithm is about 10% faster on the 800 million by 10 matrix and runs significantly faster for the 20 billion by 4 matrix. The packed rows have little effect on the running time in the 800 million by 10 case, which is in contrast to the same matrix with the Python implementation Figure 6. The algorithms both see significant

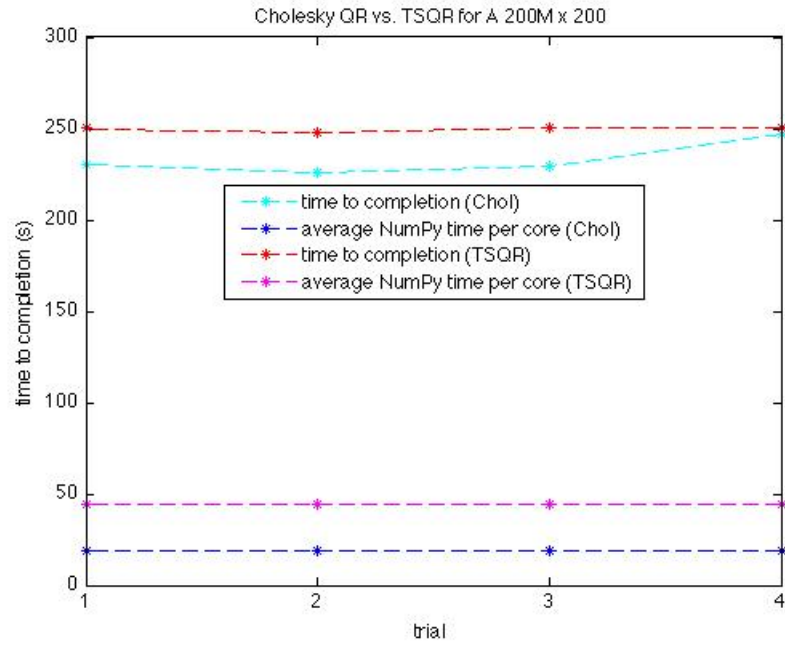


Figure 9: Python MRTSQR and MRCQR with time spent in NumPy

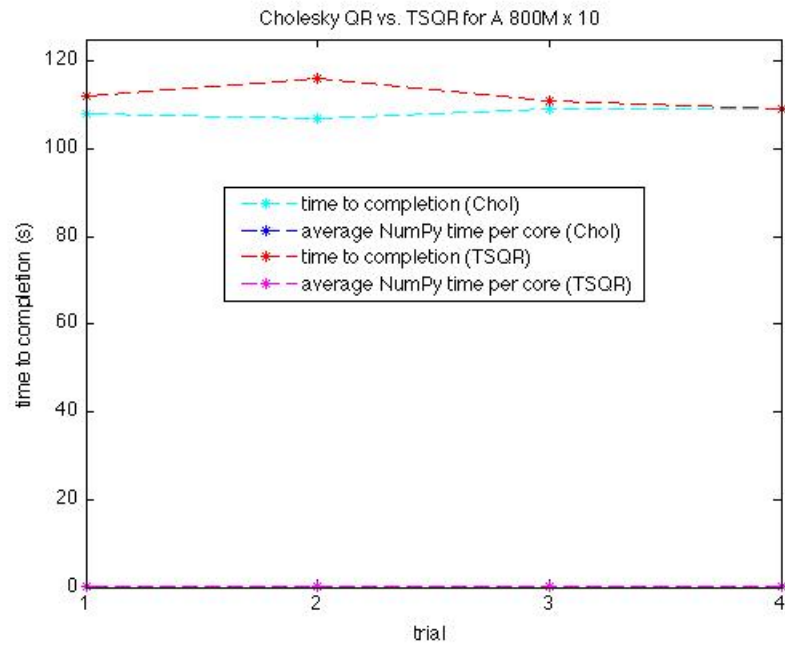


Figure 10: Python MRTSQR and MRCQR with time spent in NumPy

speedups due to the packed rows of the 20 billion by 4 matrix.

Figure 12 looks at the average LAPACK time per core, i.e. the amount of time spent in computation per core. Interestingly, the TSQR algorithm spends less time in computation than the Cholesky QR algorithm. However, we also see variations in the computation time across different packed rows. Note that the average time spent in LAPACK per core is less than 0.1 seconds in all cases, so variations could be due to errors in timing, or function call overhead. The Cholesky QR algorithm makes several thousand more calls to LAPACK. The algorithm calls `dsyrk` for $A^T A$, `daxpy` for row sums, and `dpotrf` for Cholesky. TSQR only makes calls to `dgeqrf`.

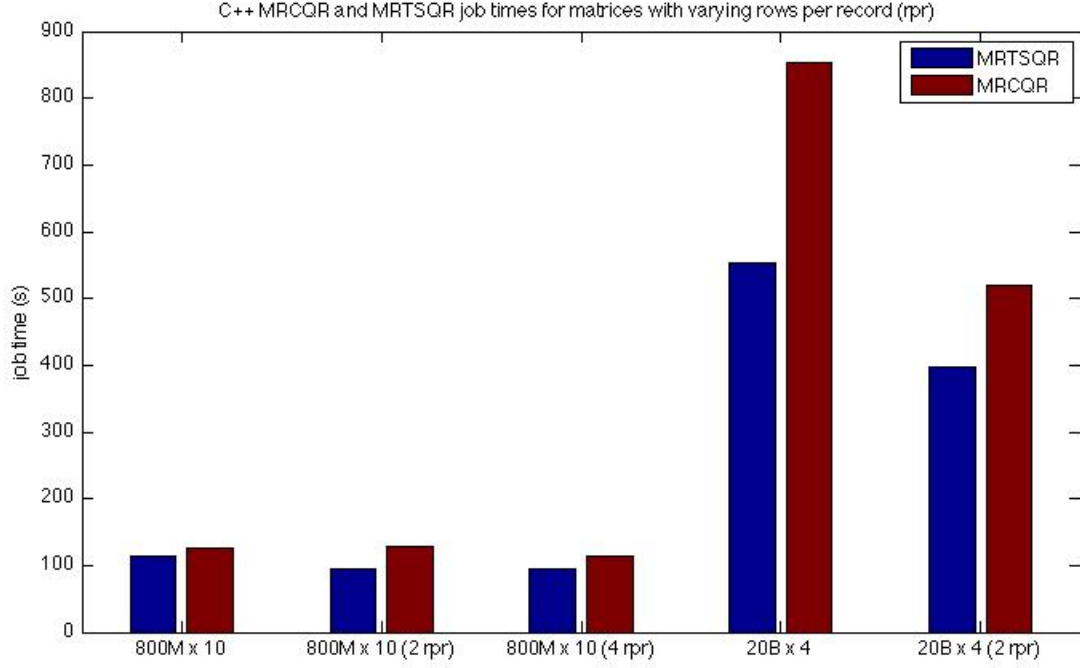


Figure 11: C++ MRTSQR and MRCQR total job times

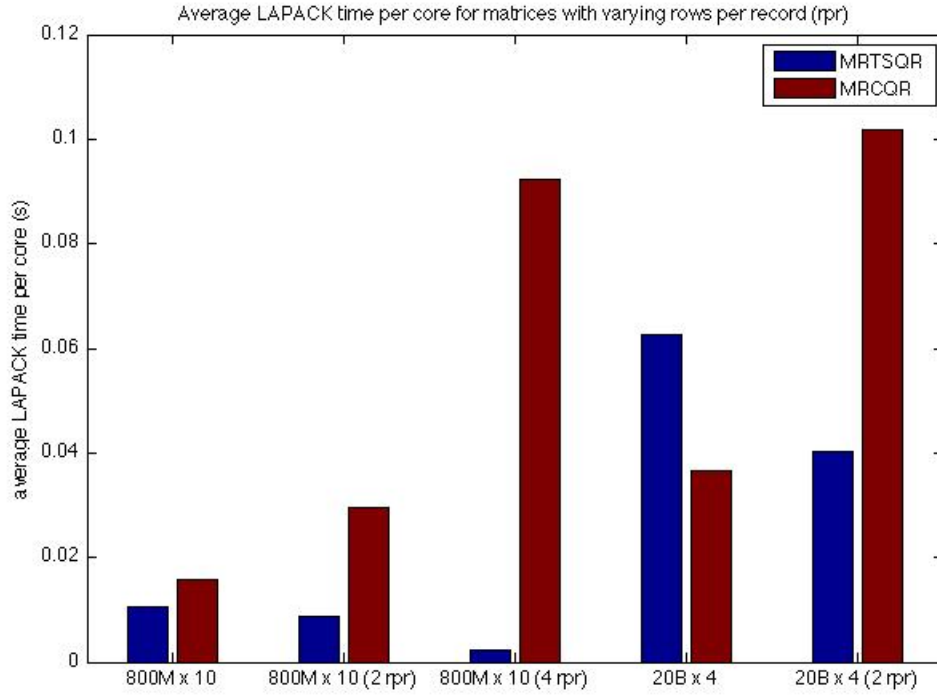


Figure 12: C++ MRTSQR and MRCQR time spent in LAPACK

Figure 13 compares the total running times of the C++ and Python implementations of TSQR on two matrices (800 million by 10 and 200 million by 200). For the 800 million by 10 matrix, the implementations achieve similar performance. For the 200 million by 200 matrix, the implementations vastly differ in performance. The C++ implementation runs approximately four times faster than the Python implementation.

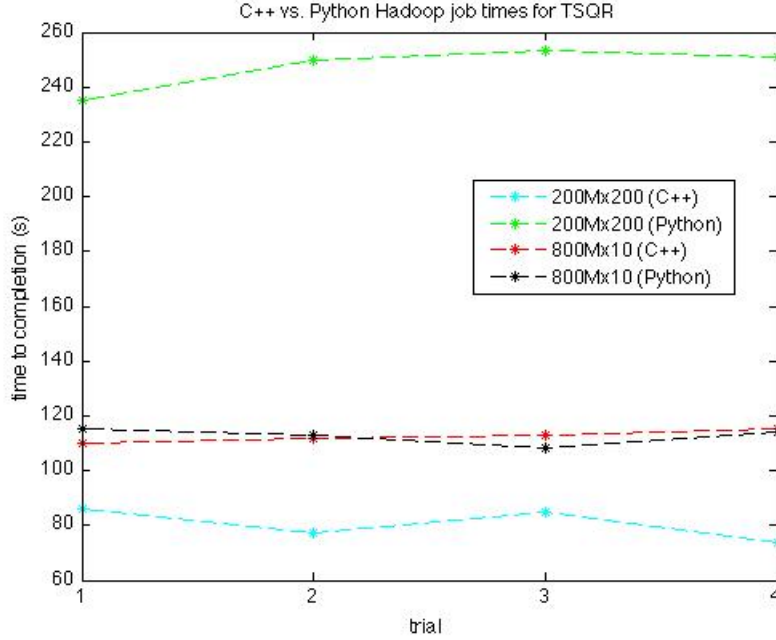


Figure 13: C++ and Python time for a 800M by 10 matrix

7.2 Benchmarking Hadoop overhead

One way of measuring Hadoop overhead is to spawn a large job on a small input. In this experiment, we have a simple two-iteration MapReduce job with an input size of approximately 1 KB:

$$(k, v) \xrightarrow[\text{max}]{\text{identity}} (k, v) \xrightarrow[\text{max}]{\text{identity}} (k, v) \xrightarrow[\text{max}]{\text{identity}} (k, v) \xrightarrow[1]{\text{identity}} (k, v).$$

The first iteration uses the maximum available map and reduce tasks. The second iteration uses the maximum available map tasks and one reduce task. An experiment with this data is given in Table 1.

Table 1: Running times of identity map and reduce tasks

trial	first iteration time (s)	second iteration time (s)	total time (s)
1	35	32	67
2	42	31	73
3	36	31	67
4	33	31	64
5	34	34	68

It takes a little over a minute just to launch the two-step iterative Hadoop jobs. Based on results earlier in the section, this ranges from 20-50% of running time.

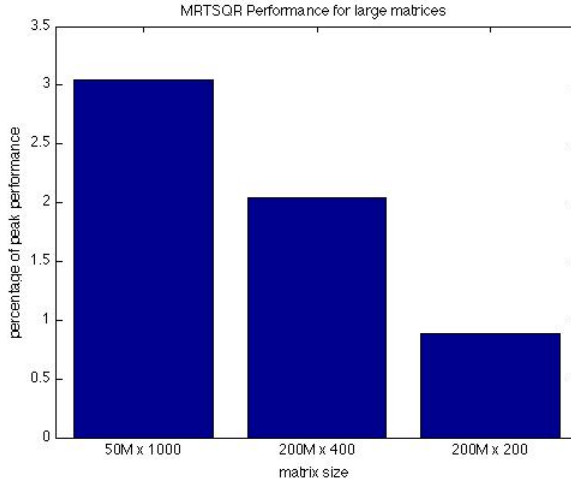
7.3 Peak performance

We look at the performance as a fraction of peak. In particular, we look at three large matrices. The sizes of the sample matrices and the running time of the TSQR algorithm is given in Table 2.

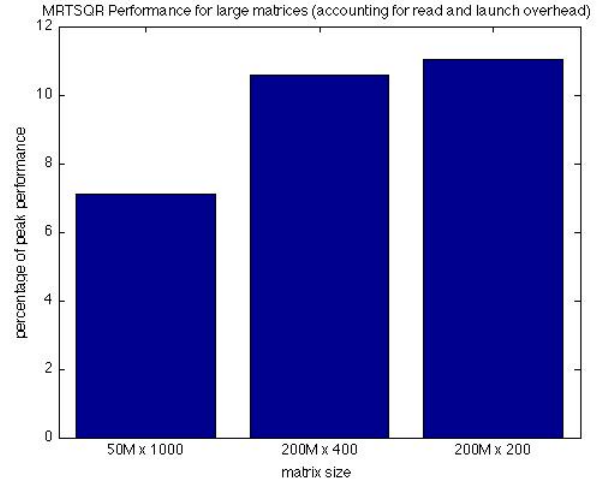
Figure 14 shows the performance of TSQR on these algorithms as a fraction of the peak performance of the machine. The peak performance of the machine is $\#(\text{nodes}) \times 85$ GFlops. In this case we have 76 nodes, so peak performance is 6460 GFlops. Figure 14a shows the raw fraction of peak, which includes all of the Hadoop overhead and disk reads. We get 1-3% of peak for these matrices. Figure 14b shows the fraction of peak, after removing 60 seconds for Hadoop overhead and accounting for 60 MB/s reads. 50-60 MB/s sequential disk reading was an estimate given by NERSC. With this simple accounting, we get 7-11% peak. This is strong performance for a MapReduce architecture.

Table 2: Performance of three large matrices using C++ TSQR on 76 nodes

m	n	size of matrix (GB)	GFlops	Running time (1 st iteration) (s)	Running time (2 nd iteration) (s)
50M	1000	372.53	199.20	166	85
200M	400	596.05	133.33	207	33
200M	200	298.02	57.97	108	30



(a) Raw performance



(b) Accounting for launch, cleanup, and disk read overhead

Figure 14: Measuring performance by fraction of peak

8 Numerical stability

In order to test numerical stability, we can strategically pick our matrix A to control its condition number. We start with a m by n matrix A' with matrix entries taken from $N(0,1)$. Then

we compute $A' = Q'R'$. Q' also has matrix entries from $N(0,1)$. Let D be a diagonal matrix with $D_{jj} > 0$. We then take a n by n matrix \tilde{A} with matrix entries from $N(0,1)$ and compute $\tilde{A} = \tilde{Q}\tilde{R}$. Finally, let $A = Q'D\tilde{Q}$. This is precisely the SVD of A , so we get the condition number by:

$$\kappa(A) = \frac{\sigma_{max}}{\sigma_{min}} = \frac{\max_j D_{jj}}{\min_j D_{jj}} [9].$$

For numerical stability experiments, we simply vary the matrix D to control the condition number. To evaluate the stability of the algorithm we compute $\|Q^T Q - I_n\|_2$, i.e. how orthogonal is the computed Q . To get Q , we form R^{-1} and take $Q = AR^{-1}$. Computing R^{-1} is not stable. If Q is not quite orthogonal, we can perform another QR decomposition to reduce the error. This strategy is called iterative refinement [9]. The idea is shown in equation 9:

$$A = \hat{Q}\hat{R} = (\hat{Q}'\hat{R}')\hat{R} \tag{9}$$

If \hat{Q} is orthogonal (as it would be in exact arithmetic), then $\hat{Q}' = \hat{Q}$ and $\hat{R}' = I_n$.

Figures 15 and 16 show the results of a number of experiments with varying $\kappa(A)$. Figure 15 shows the error for a small matrix (1000 by 10), where the algorithms were run locally on a single processor. We see the effects of the squaring of the condition number in Cholesky QR. After one step of iterative refinement, the errors are close ϵ_{mach} . Figure 16 shows the error for a large matrix (100 million by 10), where the algorithms were run on the entire cluster with 600 processors. Here, we see the same effects, except that one step of iterative refinement with Cholesky QR does not reduce the error as much.

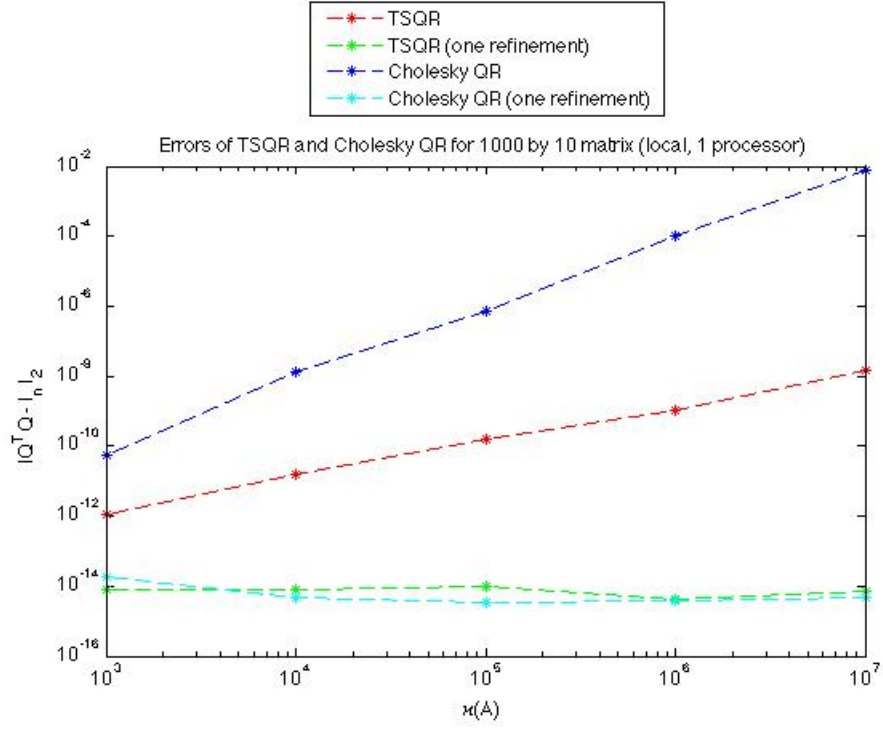


Figure 15: Errors of TSQR and Cholesky with iterative refinement (1000 by 10 matrix)

8.1 MapReduce scheme for $Q = AR^{-1}$

Our MapReduce scheme for $Q = AR^{-1}$ assumes that we have already computed R . The R matrix gets distributed to every map task, and the rows of A get distributed to the mappers:

$$(k, A_i) \xrightarrow[\text{max}]{AR^{-1}} (k, Q_i) \xrightarrow[\text{max}]{\text{identity}} (k, Q_i)$$

We only need one iteration because the entire computation is embarrassingly parallel, and we can leave the resulting Q matrix splayed across multiple directories. A visual representation of the scheme is in Figure 17.

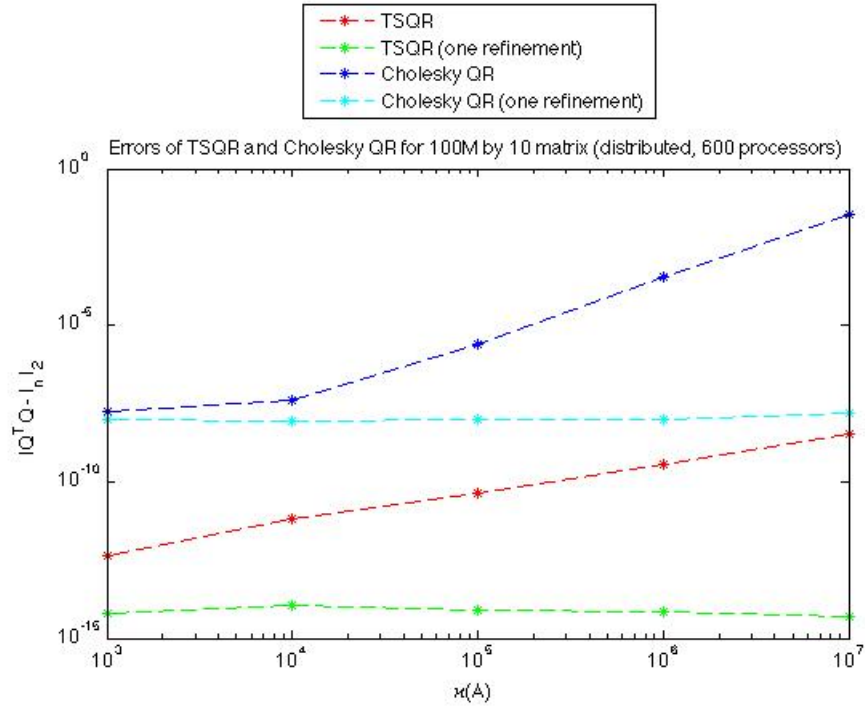


Figure 16: Errors of TSQR and Cholesky with iterative refinement (100,000,000 by 10 matrix)

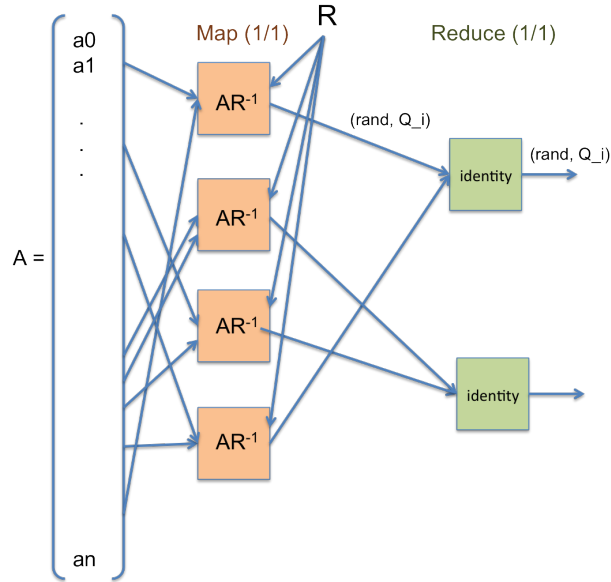


Figure 17: $Q = AR^{-1}$ scheme

9 Fault tolerance

The central benefit to scientific computing in cloud environments is stability. In Hadoop, failed tasks are restarted 3 times by default, and this is a tunable parameter [11]. This provides the user with the comfort that a single point of failure will not derail entire jobs. Furthermore, consistently failing nodes are “blacklisted” and not included in future jobs.

With supercomputers moving towards exascale, fault tolerance is becoming increasingly important [5]. We hope that the experiments discussed in this section reinforce the idea that we do not need to worry too much about faults affecting performance. To benchmark performance penalties, random software faults were introduced in the MRTSQR algorithm, and the performance was evaluated as the fault rate increased. Faults were introduced in three different ways: (1) in both map and reduce tasks, (2) only in map tasks, and (3) only in reduce tasks.

Figure 18 shows the results for case (1), where faults were simulated in both map and reduce tasks. The dashed lines are a reference for the running time with no faults. For the 200 million by 200 matrix, there were around 3000 tasks, and for the 800 million by 800 matrix, there were around 1000 tasks. On the left-hand side, we have a $P(\text{fault}) = \frac{1}{5}$, and the performance penalty is approximately 50%. This demonstrates the reliability of Hadoop: even with one in five tasks failing, we still finish the job relatively quickly.

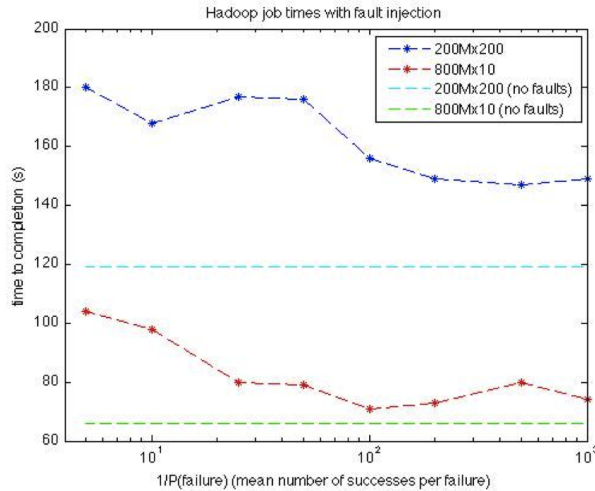


Figure 18: Measuring performance penalties induced by simulated faults in map and reduce tasks

Figure 19 shows results for cases (1), (2), and (3), where each experiment was run independently. As expected, map-only and reduce-only fault scenarios incur a noticeably smaller penalty in most cases. However, the noise in the data does not allow us to differentiate the effects of map faults and reduce faults when they are both present in the system.

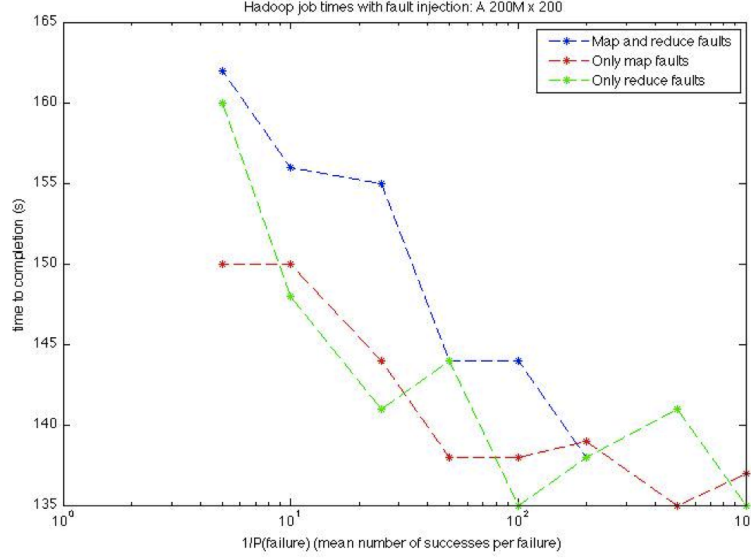


Figure 19: Measuring performance penalties induced by simulated faults in map and reduce tasks

10 Strong scaling in the cloud

Strong scaling with Hadoop is a challenge as map tasks are provided on an as-available basis, rather than an as-needed basis. In other words, map resources are greedily consumed. In order to control the number of map tasks, we can manipulate the `mapred.min.split.size` parameter, which sets the minimum number of bytes for a given map task to consume as input.

Figure 20 shows the amount of time for a job and the amount of average time spent in NumPy per core as a function of the number of nodes. The average time spent in NumPy per core was calculated by having a Hadoop counter incremented by each task with the time spent in computation. This time was then divided by the total number of cores. The plot shows two important trends. First, the average time spent in NumPy per core is much smaller than the total job time. This is especially true for the 800 million by 100 matrix. This makes sense as we expect communication overheads to be higher with smaller rows and with more rows.

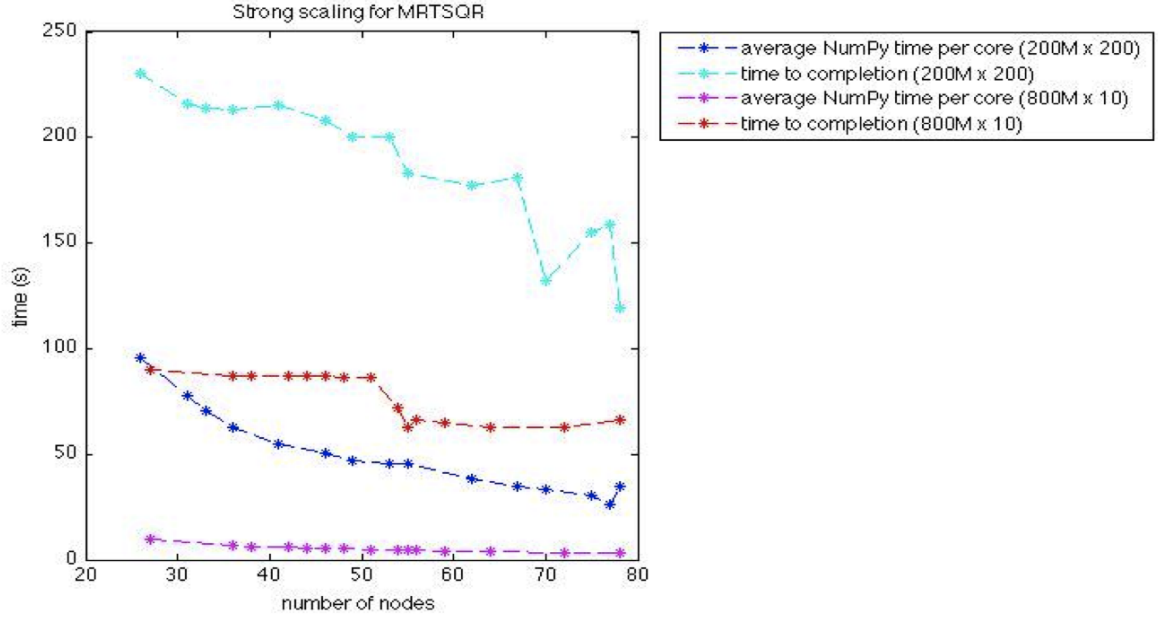


Figure 20: Strong scaling of Householder TSQR

11 Future work

There is not much room for optimizations to the TSQR codes, but there is large room for expanding the scope of MapReduce to other problems in numerical linear algebra and applied mathematics. One possible optimization would be a customized storage format for reading and writing raw bytes. A Java implementation would be interesting because we would no longer need Hadoop streaming, but Java linear algebra libraries are less cooperative than the analogous libraries in C++ and Python.

A major project would be extracting the matrix Q by storing the intermediate Q from local QR decompositions. This is a challenging undertaking because we have to store intermediate states in the cloud. It would be interesting to see the MapReduce paradigm applied to other linear algebra problems. LU is a candidate here. Tensor algebra also provides new opportunities. Unrolling higher-dimensional matrices to 2D tall-and-skinny matrices could provide interesting results.

12 Conclusion

We can process 500 GB matrices in 2-3 minutes on about 75 nodes with a simple programming model. Furthermore, we gain fault tolerance. For these reasons, numerical linear algebra in the cloud with MapReduce is an attractive option for computational science. Python allows for simple prototyping, which is difficult to achieve for general high-performance computing codes. C++ allows us to optimize these prototypes. With a liberal performance model, we can get around 1-3% peak, which is good for disk-based IO. In basic use cases, MRTSQR is a better choice than MRCQR. However, having both options could be useful for other matrices. MRTSQR is superior

in terms of numerical stability, as expected.

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References

- [1] The Apache Software Foundation. MapReduce Tutorial. 2008.
〈 http://hadoop.apache.org/common/docs/current/mapred_tutorial.html 〉
- [2] Austin Benson. MapReduce TSQR code. 〈 <https://github.com/arbenson/mrtsqr> 〉
- [3] Klaas Bosteele. TypedBytes. 〈 <https://github.com/klbostee/typedbytes> 〉
- [4] Klaas Bosteele. Dumbo. 〈 <https://github.com/klbostee/dumbo> 〉
- [5] Franck Cappello. Fault Tolerance in Petascale/Exascale Systems: Current Knowledge, Challenges and Research Opportunities. *The International Journal of High Performance Computing Applications* 23.3, (2009): 212–222.
- [6] Paul G. Constantine and David F. Gleich. Tall and skinny QR factorizations in MapReduce architectures. In *Proceedings of the second international workshop on MapReduce and its applications*, MapReduce '11, pages 43–50, New York, NY, USA, 2011. ACM.
- [7] Shane Corder. High Performance Linpack on Xeon 5500 v. Opteron 2400. 16 June 2009. 〈 <http://www.advancedclustering.com/company-blog/high-performance-linpack-on-xeon-5500-v-opteron-2400.html> 〉. Accessed 11 November 2011.
- [8] James Demmel, Laura Grigori, Mark F. Hoemmen, and Julien Langou. Communication-optimal parallel and sequential QR and LU factorizations. UCB/EECS-2008-89. August 2008.
- [9] James Demmel. Applied Numerical Linear Algebra. SIAM. 1997.
- [10] David Gleich. MapReduce TSQR code. 〈 <https://github.com/dgleich/mrtsqr> 〉
- [11] Hadoop version 0.20. 〈 <http://hadoop.apache.org/> 〉
- [12] Hadoop Wiki: PoweredBy. 〈 <http://wiki.apache.org/hadoop/PoweredBy> 〉
- [13] Herodotos Herodotou. Hadoop Performance Models. Technical Report, CS-2011-05. Duke University. May 2011.
- [14] Magellan at NERSC. 〈 <http://magellan.nersc.gov> 〉
- [15] Eric Jones, Travis Oliphant, Pearu Peterson and others. SciPy: Open Source Scientific Tools for Python. 2001. 〈 <http://www.scipy.org> 〉