CS 598: Communication Cost Analysis of Algorithms

Lecture 8: scalable QR factorization of rectangular matrices

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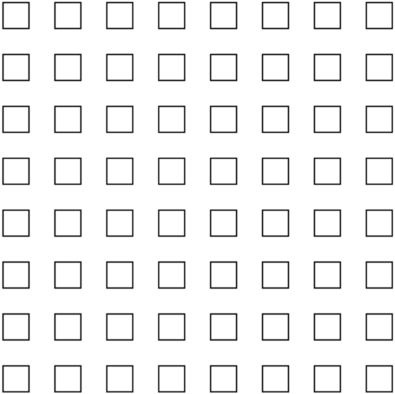
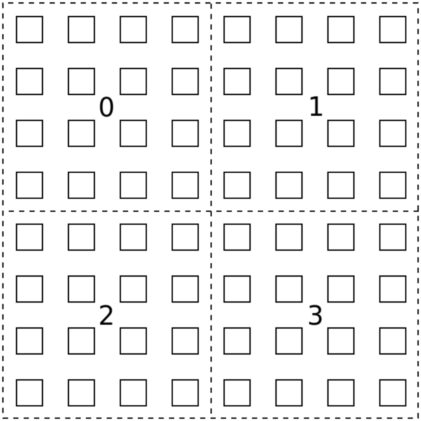
Matrix



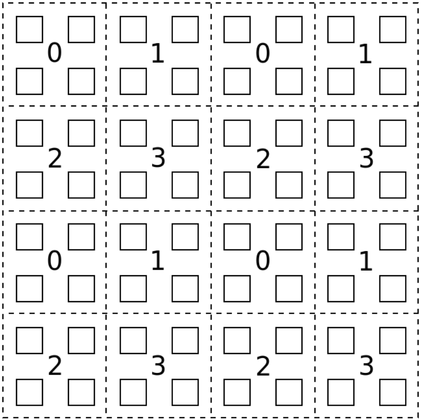
16-by-16 matrix

Blocked layout



blocked layout

Block-cyclic layout



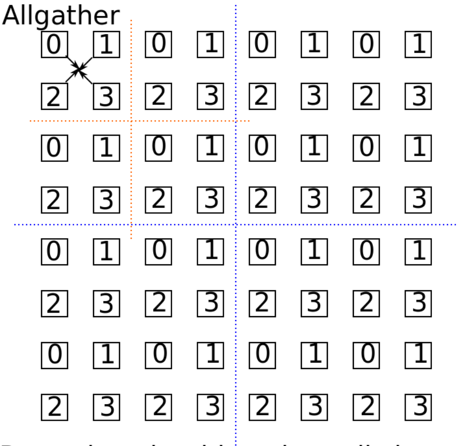
block-cyclic layout

Cyclic layout

0	1	0	1	0	1	0	1
2	3	2	3	2	3	2	3
0	1	0	1	0	1	0	1
2	3	2	3	2	3	2	3
0	1	0	1	0	1	0	1
2	3	2	3	2	3	2	3
0	1	0	1	0	1	0	1
2	3	2	3	2	3	2	3

cyclic layout

Recursion with cyclic layout



Recursive algorithms in cyclic layout

All processors work until base-case

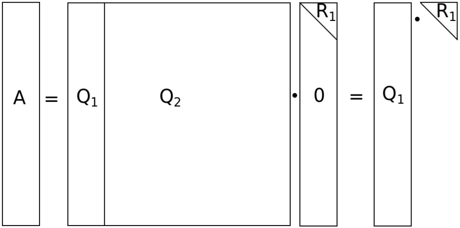
$$T(n,P) = 2T(n/2,P) + O(\alpha \cdot \log(P) + n^2/P \cdot \beta),$$

$$T(n_0,P) = O(\alpha \cdot \log(P) + n_0^2 \cdot \beta)$$

Rectangular QR

Consider QR factorization of $m \times n$ matrix A when $m \geq n$

- so far we have focused on $m = n$
- we will first consider $m \geq nP$, then the more general case
- we can decompose Q and R in $A = QR$ as follows



- Q: given $Q_1 R_1 = A$ and $Q_1^T Q_1 = I$, would choosing $Q_2 = 0$ yield a valid QR decomposition of A?
- A: no, it would not satisfy the orthogonality criterion, $Q^T Q = I$
- we need $Q_1 Q_2^T = 0$ and $Q_2 Q_2^T = I$; given Q_1, Q_2 is not unique

Rectangular QR for least squares

Given $m \times n$ matrix A with $m \leq n$, compute $\text{argmin}_{x \in \mathbb{R}^n}(||Ax - b||_2)$

- solve $Rx = Q^T b$, i.e. $x = R^+ Q^T b$
- $R^+ = [R_1^{-1} \ \ 0]$ where R_1 is $n \times n$
- Q: given Q_1 (the first n columns of Q), do we need Q_2?
- A: No, since, $Q^T b = \begin{bmatrix} Q_1^T b \\ Q_2^T b \end{bmatrix}$ and $[R_1^{-1} \ \ 0] \begin{bmatrix} Q_1^T b \\ Q_2^T b \end{bmatrix} = R_1^{-1} Q_1^T b$
- rectangular QR factorizations are also used in iterative methods such as block-Arnoldi (orthogonalization is used implicitly in many others)
- in these methods it typically suffices to have Q_1

Rectangular QR within square QR

QR of tall and skinny matrices is also a subroutine in square matrix factorizations

- in the last lecture, we utilized QR factorizations of matrix panels within 2D QR
- panel QR factorizations are also done for SVD and eigenvalue decompositions
- in the case of 2D QR, we apply the full $m \times m$ transformation Q^T
- Q: what representation could we use for Q computed from an $m \times n$ matrix A, to compute $Q^T B$ where B is $n \times k$, with mnk computation?
- A: Householder: $Q = (I - YTY^T)$, where Y is $m \times n$

Tall-skinny QR (TSQR)

Given an $m \times n$ matrix A, distributed over P processors so that $\Pi(i)$ owns $A(in/P + 1 : (i+1)n/P, :)$

- we can use Householder QR, but this requires $n \log(P)$ synchronizations
- there are a few alternative algorithms that achieve require $O(\log(P))$ synchronizations
- the simplest is probably Cholesky-QR
  - compute symmetric matrix $B = A^T A$
  - factorize B using Cholesky $B = LL^T = R_1^T R_1$
  - perform 'TRSM' (back-substitution) $Q_1 = AR_1^{-1}$
  - cheap but not stable, $\text{cond}(B) = \text{cond}(A)^2$, so radical instability when $\text{cond}(A) \geq 1/\sqrt{\epsilon_{\text{mach}}}$
  - orthogonality of Q is often poor

Cholesky QR2

Cholesky-QR can be made more stable [Yamamoto et al 2014]

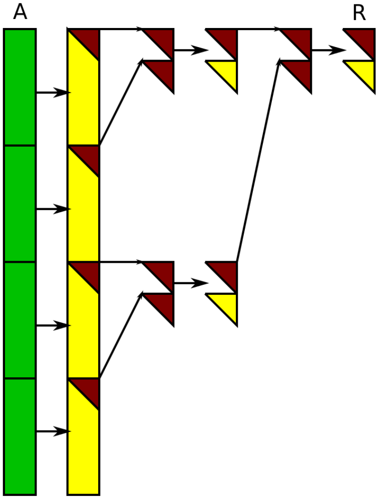
- as before, compute $\{\bar{Q}_1, \bar{R}_1\} = \text{Cholesky-QR}(A)$
- then, iterate! $\{Q_1, \hat{R}_1\} = \text{Cholesky-QR}(\bar{Q}_1)$
- $R_1 = \hat{R}_1 \bar{R}_1$
- $A = Q_1 R_1$
- solution still bad when $\text{cond}(A) \geq 1/\sqrt{\epsilon_{\text{mach}}}$
- but if $\text{cond}(A) < 1/\sqrt{\epsilon_{\text{mach}}}$, it is numerically stable because $\text{cond}(\bar{Q}_1) \approx 1$
- parallel Cholesky-QR2
  1. perform $A^T A$ using an allreduce of size $n^2/2$
  2. compute Cholesky redundantly and TRSM to get $\bar{Q}_1$ and $\bar{R}_1$
  3. perform $\bar{Q}_1^T \bar{Q}_1$ using an allreduce of size $n^2/2$
  4. compute Cholesky redundantly, TRSM, and $R_1 = \hat{R}_1 \bar{R}_1$ to get Q_1, R_1
  5. $T_{\text{Cholesky-QR2}}(m, n, P) = 2T_{\text{allred}}(n^2/2, P) = 2n^2 \cdot \beta + 4\log_2(P) \cdot \alpha$
- for QR of a tall-skinny A with $\text{cond}(A) < 1/\sqrt{\epsilon_{\text{mach}}}$, this algorithm is trivial to implement, stable, and very fast

Recursive TSQR

Block Givens rotations yield another idea

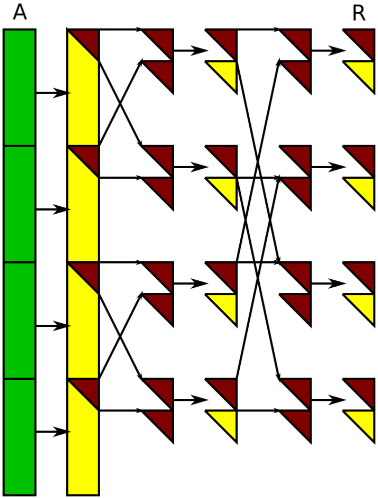
- we can also employ a recursive scheme analogous to tournament pivoting for LU
- subdivide $A = \begin{bmatrix} A_\text{U} \\ A_\text{L} \end{bmatrix}$ and recursively compute $\{Q_\text{U}, R_\text{U}\} = \text{QR}(A_\text{U})$, $\{Q_\text{L}, R_\text{L}\} = \text{QR}(A_\text{L})$ concurrently with $P/2$ processors each
- we have $A = \begin{bmatrix} Q_\text{U} R_\text{U} \\ Q_\text{L} R_\text{L} \end{bmatrix} = \begin{bmatrix} Q_\text{U} & 0 \\ 0 & Q_\text{L} \end{bmatrix} \begin{bmatrix} R_\text{U} \\ R_\text{L} \end{bmatrix}$
- (all)gather R_U and R_L and compute sequentially, $\begin{bmatrix} R_\text{U} \\ R_\text{L} \end{bmatrix} = \tilde{Q} R$
- we now have $A = QR$ where $Q = \begin{bmatrix} Q_\text{U} & 0 \\ 0 & Q_\text{L} \end{bmatrix} \tilde{Q}$

Recursive TSQR, binary tree (binomial comm. pattern)



Householder vectors are denoted in yellow (R is R_1)

Recursive TSQR, butterfly, redundant R computation



Householder vectors are denoted in yellow (R is R_1)

Cost analysis of recursive TSQR, butterfly

We can subdivide the cost into base cases (tree leaves) and internal nodes

- let the cost per flop be γ
- every processor computes a QR of their $m/P \times n$ leaf matrix block

$$T_{\text{Rec-TSQR}}(m_0, n, 1) = m_0 n^2 \cdot \gamma$$

- Q: what cost do we incur at every tree node

$$T_{\text{Rec-TSQR}}(m, n, P) = T_{\text{Rec-TSQR}}(m/2, n, P/2) + O(?)$$

- A: $O(n^3 \cdot \gamma + n^2 \cdot \beta + \alpha)$, for a total cost of

$$T_{\text{Rec-TSQR}}(m, n, P) = O([mn^2/P + n^3 \log(P)] \cdot \gamma + n^2 \log(P) \cdot \beta + \log(P) \cdot \alpha)$$

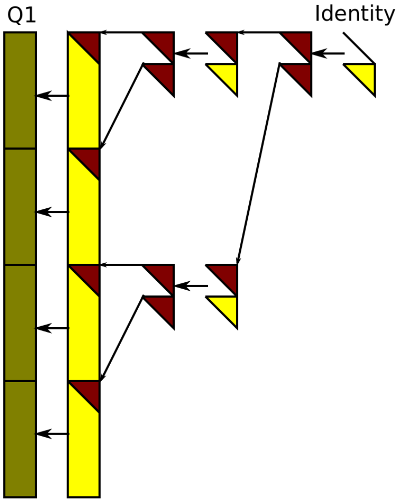
- Q: How does this bandwidth cost compare to Cholesky-QR2?
- Hint: the communication cost of Cholesky-QR2 is $2T_{\text{allreduce}}(n^2/2, P)$
- A: The cost of recursive TSQR is a factor of $O(\log(P))$ greater.

Computing Q_1 in recursive TSQR

Lets now consider how to compute the $m \times n$ set of orthonormal columns Q_1 such that $A = Q_1 R_1$ for $n \times n$ upper-triangular R_1

- we had the recurrence $Q = \begin{bmatrix} Q_U & 0 \\ 0 & Q_L \end{bmatrix} \tilde{Q}$
- these orthogonal factors: Q_L, Q_U, $\tilde{Q}$ have a lot of structure, especially if represented with Householder vectors or Givens rotations
- Q: how do we compute Q when performing regular Givens rotations?
- A: by applying them to an identity matrix, similar idea here...
- instead of computing the full $m \times m$ matrix Q (which really, we never want explicitly), we can apply the implicit representation of Q to $\begin{bmatrix} I \\ 0 \end{bmatrix}$ where I is $n \times n$ to get Q_1
- this has the same cost as the tree for computing R, except now we do it backwards

Computing Q_1 in recursive TSQR



Short pause

Homeworks and projects

- any questions on homework problems?
- office hours Tuesday 3-4
- posts on Piazza on late Tuesday evening may not get a response until Wednesday morning
- first project proposal due Sep 28th, email me or stop by to discuss preliminary ideas

Recursive TSQR within a 2D algorithm

Consider using recursive TSQR for $n \times b$ panel factorizations to factorize an $n \times n$ matrix using a 2D algorithm

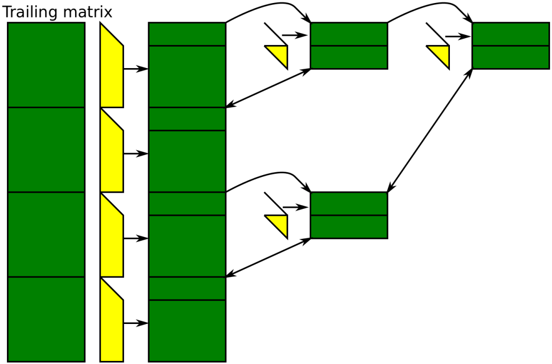
- each of n/b TSQRs would have cost

$$T_{\text{Rec-TSQR}}(n, b, \sqrt{P}) = O(b^2 \log(P) \cdot \beta + \log(P) \cdot \alpha)$$

- Q: if we want to achieve a bandwidth cost of $O(n^2/\sqrt{P} \cdot \beta)$ in the entire 2D algorithm, how does Rec-TSQR restrict our choice of b?
- A: $b \leq \frac{n}{\sqrt{P}\log(P)}$
- to perform trailing matrix updates, we need to multiply by Q^T, where we can again use its implicit tree representation
- Q: would we need to traverse the tree from the leaves to the root, as we did when computing R, or from the root to the leaves as we did for computing Q_1?
- A: from the leaves to the root, since

$$Q^T = \left(\begin{bmatrix} Q_\text{U} & 0 \\ 0 & Q_\text{L} \end{bmatrix} \tilde{Q} \right)^T = \tilde{Q}^T \begin{bmatrix} Q_\text{U}^T & 0 \\ 0 & Q_\text{L}^T \end{bmatrix}$$

Apply implicit Q^T via binary tree



Cost analysis of applying Q^T via binary tree

We need to apply Q^T for each panel, n/b times

- every time, we need to update up to $n - b = O(n)$ columns
- the cost of the update done in the tree leaves is

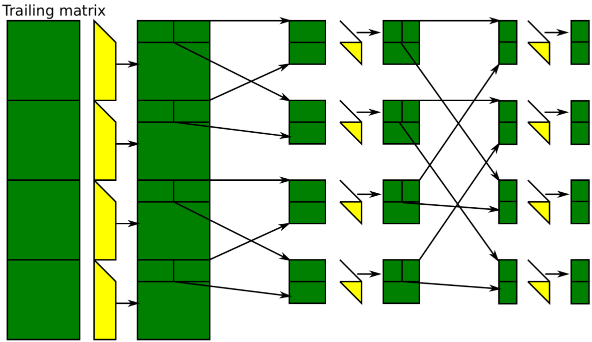
$$O\Big(\frac{n^2 b}{P} \cdot \gamma + \frac{nb}{\sqrt{P}} \cdot \beta + \log(P) \cdot \alpha\Big)$$

- for every tree node, we need to communicate the b updated rows, a block of dimension proportional to $b \times n/\sqrt{P}$
- Q: what is then the bandwidth cost of whole tree update?
- A: $O(nb\log(P)/\sqrt{P} \cdot \beta)$, the tree nodes cost:

$$O\Big(\frac{nb^2 \log(P)}{P} \cdot \gamma + \frac{nb\log(P)}{\sqrt{P}} \cdot \beta + \log(P) \cdot \alpha\Big)$$

- since there are n/b such updates, the 2D algorithm would have a bandwidth cost of at least $O\Big(\frac{n^2 \log(P)}{\sqrt{P}} \cdot \beta\Big)$

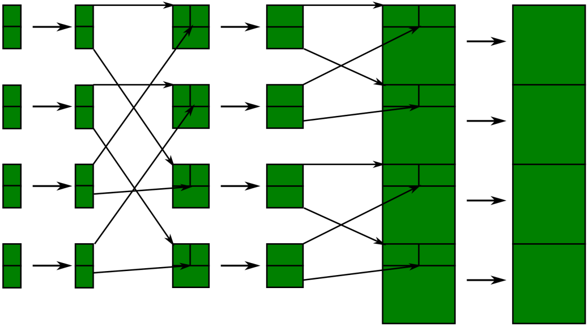
Apply implicit Q^T via butterfly



Subdivide updated columns recursively to keep all processors busy

$$T(b, n, P) = T(b, n/2, P/2) + O\left(\frac{nb^2}{P} \cdot \gamma + \beta \cdot nb/\sqrt{P} + \alpha\right)$$

Apply implicit Q^T via butterfly



After recursion, return the columns back to owner, for a total cost of

$$T(b, n, P) = O\left(\frac{nb^2}{P} \cdot \gamma + \beta \cdot nb/\sqrt{P} + \alpha \cdot \log(P)\right)$$

Motivation for Householder reconstruction

The trailing matrix update in Householder QR is still the most efficient

- consists of $O(1)$ matrix multiplications
- requires standard collective communication, rather than an algorithmic tree
- compliant with standard libraries (ScaLAPACK returns Y not Q for `dgeqrf`)
- moreover, how do we do a trailing matrix update with Cholesky-QR2?

Householder reconstruction

Given $m \times n$ matrix Q_1, we can construct Y such that $Q = (I - YTY^T) = [Q_1, Q_2]$ and Q is orthogonal

- key idea due to Yusaku Yamamoto (2013)
- note that in the Householder representation, we have $I - Q = Y \cdot TY^T$, where Y is lower-trapezoidal and TY^T is upper-trapezoidal
- let $Q_1 = \begin{bmatrix} Q_{11} \\ Q_{21} \end{bmatrix}$ where Q_{11} is $n \times n$, compute

$$\{Y, TY_1^T\} = \text{LU}\Big(\begin{bmatrix} I - Q_{11} \\ Q_{21} \end{bmatrix}\Big),$$

where Y_1 is the upper-triangular $n \times n$ leading block of Y^T

Householder reconstruction stability

Householder reconstruction can be done with unconditional stability

- we need to be just a little more careful

$$\{Y, TY_1^T\} = \mathrm{LU}\left(\begin{bmatrix} S - Q_{11} \\ Q_{21} \end{bmatrix}\right),$$

  where S is a sign matrix (each value in $\{-1, 1\}$) with values picked to match the sign of the diagonal entry within LU
- these are the sign choices we need to make for regular Householder factorization
- since all entries of Q_1 are ≤ 1, pivoting is unnecessary (partial pivoting would do nothing)
- since $\mathrm{cond}(Q) \approx 1$, Householder reconstruction is stable

Householder reconstruction for square matrix factorizations

Householder reconstruction provides a kind of abstraction between the panel factorization and trailing matrix update

- use algorithm of choice for panel QR, e.g. Cholesky-QR(2) or recursive TSQR
- construct Q_1 and reconstruct Y
  - construction of Q_1 should cost no more than the factorization itself
  - performing LU of Q_1 requires a sequential $n \times n$ LU and a broadcast of the U factor for TRSM
- now perform trailing matrix update as if we had done Householder QR
- so we can achieve same bandwidth costs as in previous lecture, but lower synchronization cost ($O(\sqrt{cP} \cdot \alpha)$)
- for recursive TSQR, extra factor of $\log(P)$ in bandwidth cost requires a block size smaller by a factor of $\log(P)$, yielding $\log(P)$ higher synchronization cost than if we use Cholesky-QR2

QR for rectangular matrices

What if we want to factorize an $m \times n$ rectangular matrix, where $m > n$, but not $m \gg n$

- TSQR algorithms have cost factors of $O(n^3 \cdot \gamma + n^2 \cdot \beta)$ or higher, which may be problematic
- 2D and 3D algorithms have assumed $m = n$
- there are a couple of alternative approaches for the general case
- intuitively, we want to use processor grids that match the dimensions of the $m \times n \times n$ problem

Elmroth-Gustavson algorithm (3Dx2Dx1D)

One approach is to use column-recursion $A = [A_1, A_2]$

- compute $\{Y_1, T_1, R_1\} = \text{QR}(A_1)$ recursively with P processors
- perform rectangular matrix multiplications with communication-avoiding algorithms to compute $B_2 = (I - Y_1 T_1 Y_1^T)^T A_2$
- compute $\{Y_2, T_2, R_2\} = \text{QR}(B_{22})$ where $B_2 = \begin{bmatrix} R_{12} \\ B_{22} \end{bmatrix}$ recursively
- concatenate Y_1 and Y_2 into Y and compute T from Y via rectangular matrix multiplication
- output $\left\{ Y, T, \begin{bmatrix} R_1 & R_{12} \\ 0 & R_2 \end{bmatrix} \right\}$
- pick an appropriate number of columns for a TSQR base-case

Elmroth-Gustavson algorithm (1Dx2Dx3D)

Another approach is to use “row-recursion”

- perform recursive TSQR, where each node in the tree is factorized with Pn/m processors (if $P \geq m/n$, a TSQR algorithm is the best option anyway)
- leaf nodes will require just a square QR
- tree nodes require QR of two stacked upper-triangular matrices
- interleave the rows of the upper-triangular matrices and you get a $2:1$ ratio, i.e. slanted panel, so can use Tiskin's QR algorithm without embedding!
- both of the proposed approaches achieve a bandwidth cost of $O\left(\left(\frac{mn^2}{P}\right)^{2/3}\log(P)\right)$ for $n \leq m \leq nP$