Parallel Numerical Algorithms

Chapter 11 – QR Factorization

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Outline

1. QR Factorization
2. Householder Transformations
3. Givens Rotations

QR Factorization

- For given $m \times n$ matrix $\boldsymbol{A}$, with $m > n$, *QR factorization* has form

$$\boldsymbol{A} = \boldsymbol{Q} \begin{bmatrix} \boldsymbol{R} \\ \boldsymbol{O} \end{bmatrix}$$

  where matrix $\boldsymbol{Q}$ is $m \times m$ and orthogonal, and $\boldsymbol{R}$ is $n \times n$ and upper triangular

- Can be used to solve linear systems, least squares problems, etc.

- As with Gaussian elimination, zeros are introduced successively into matrix $\boldsymbol{A}$, eventually reaching upper triangular form, but using orthogonal transformations instead of elementary eliminators

Methods for QR Factorization

- Householder transformations (elementary reflectors)
- Givens transformations (plane rotations)
- Gram-Schmidt orthogonalization

Householder Transformations

- *Householder transformation* has form

$$\boldsymbol{H} = \boldsymbol{I} - 2\frac{\boldsymbol{v}\boldsymbol{v}^T}{\boldsymbol{v}^T\boldsymbol{v}}$$

  where $\boldsymbol{v}$ is nonzero vector
- From definition, $\boldsymbol{H} = \boldsymbol{H}^T = \boldsymbol{H}^{-1}$, so $\boldsymbol{H}$ is both orthogonal and symmetric
- For given vector $\boldsymbol{a}$, choose $\boldsymbol{v}$ so that

$$\boldsymbol{H}\boldsymbol{a} = \begin{bmatrix} \alpha \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \alpha \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \alpha \boldsymbol{e}_1$$

Householder Transformations

- Substituting into formula for $\boldsymbol{H}$, we see that we can take

$$\boldsymbol{v} = \boldsymbol{a} - \alpha \boldsymbol{e}_1$$

and to preserve norm we must have $\alpha = \pm\|\boldsymbol{a}\|_2$, with sign chosen to avoid cancellation

Householder QR Factorization

for $k = 1$ **to** n

$$\alpha_k = -\text{sign}(a_{kk})\sqrt{a_{kk}^2 + \cdots + a_{mk}^2}$$

$$\boldsymbol{v}_k = \begin{bmatrix} 0 & \cdots & 0 & a_{kk} & \cdots & a_{mk} \end{bmatrix}^T - \alpha_k \boldsymbol{e}_k$$

$$\beta_k = \boldsymbol{v}_k^T \boldsymbol{v}_k$$

if $\beta_k = 0$ **then**

continue with next k

for $j = k$ **to** n

$$\gamma_j = \boldsymbol{v}_k^T \boldsymbol{a}_j$$

$$\boldsymbol{a}_j = \boldsymbol{a}_j - (2\gamma_j/\beta_k)\boldsymbol{v}_k$$

end

end

Parallel Householder QR

- Householder QR factorization is similar to Gaussian elimination for LU factorization
- Forming Householder vector $\boldsymbol{v}_k$ is analogous to computing multipliers in Gaussian elimination
- Subsequent updating of remaining unreduced portion of matrix is also analogous to Gaussian elimination
- Thus, parallel implementation is similar to parallel LU, but with Householder vectors broadcast horizontally instead of multipliers
- For this reason, we will not go into details

Givens Rotations

- *Givens rotation* operates on pair of rows to introduce single zero
- For given 2-vector $\boldsymbol{a} = [a_1 \;\; a_2]^T$, if

$$c = \frac{a_1}{\sqrt{a_1^2 + a_2^2}}, \qquad s = \frac{a_2}{\sqrt{a_1^2 + a_2^2}}$$

  then

$$\boldsymbol{Ga} = \begin{bmatrix} c & s \\ -s & c \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} \alpha \\ 0 \end{bmatrix}$$

- Scalars c and s are cosine and sine of angle of rotation, and $c^2 + s^2 = 1$, so $\boldsymbol{G}$ is orthogonal

Givens QR Factorization

- Givens rotations can be systematically applied to successive pairs of rows of matrix $\boldsymbol{A}$ to zero entire strict lower triangle
- Subdiagonal entries of matrix can be annihilated in various possible orderings (but once introduced, zeros should be preserved)
- Each rotation must be applied to all entries in relevant pair of rows, not just entries determining c and s
- Once upper triangular form is reached, product of rotations, $\boldsymbol{Q}$, is orthogonal, so we have QR factorization of $\boldsymbol{A}$

Parallel Givens QR Factorization

- With 1-D partitioning of A by columns, parallel implementation of Givens QR factorization is similar to parallel Householder QR factorization, with cosines and sines broadcast horizontally and each task updating its portion of relevant rows
- With 1-D partitioning of A by rows, broadcast of cosines and sines is unnecessary, but there is no parallelism unless multiple pairs of rows are processed simultaneously
- Fortunately, it is possible to process multiple pairs of rows simultaneously without interfering with each other

Parallel Givens QR Factorization

- Stage at which each subdiagonal entry can be annihilated is shown here for 8×8 example

$$\begin{bmatrix} \times & & & & & & & \\ 7 & \times & & & & & & \\ 6 & 8 & \times & & & & & \\ 5 & 7 & 9 & \times & & & & \\ 4 & 6 & 8 & 10 & \times & & & \\ 3 & 5 & 7 & 9 & 11 & \times & & \\ 2 & 4 & 6 & 8 & 10 & 12 & \times & \\ 1 & 3 & 5 & 7 & 9 & 11 & 13 & \times \end{bmatrix}$$

- Maximum parallelism is $n/2$ at stage $n-1$ for $n \times n$ matrix

Parallel Givens QR Factorization

- Communication cost is high, but can be reduced by having each task initially reduce its entire local set of rows to upper triangular form, which requires no communication
- Then, in subsequent phase, task pairs cooperate in annihilating additional entries using one row from each of two tasks, exchanging data as necessary
- Various strategies can be used for combining results of first phase, depending on underlying network topology
- With hypercube, for example, final upper triangular form can be reached in $\log p$ combining steps

Parallel Givens QR Factorization

- With 2-D partitioning of A, parallel implementation combines features of 1-D column and 1-D row algorithms
- In particular, sets of rows can be processed simultaneously to annihilate multiple entries, but updating of rows requires horizontal broadcast of cosines and sines

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