

Rank Revealing QR Methods for Sparse Block Low Rank Solvers

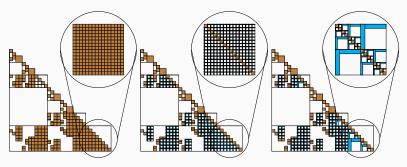
Esragul Korkmaz, Mathieu Faverge, Grégoire Pichon, Pierre Ramet 27 June 2019 – Compas

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Background

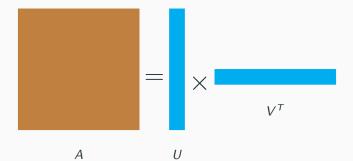
Background - ANR SaSHiMi Project

ANR SASHIMI Project



- With: Mathieu Faverge, Pierre Ramet, Grégoire Pichon
- General Picture: Solve linear equations Ax=b for large sparse systems
- Full Rank Format: Too much memory usage
- Block Low Rank Format: Compression is possible, so less storage and faster
- Hierarchical Format: Even less computational complexity and memory consumption

Background - Block Low Rank Structure



 $A \in \mathbb{R}^{m \times n}$; $U \in \mathbb{R}^{m \times r}$; $V \in \mathbb{R}^{n \times r}$

- Compression reduces memory and cost of computations
- SVD is the most accurate with lowest rank: $A_{m imes n} = \hat{U}_{m imes m} \Sigma_{m imes n} \hat{V}_{n imes n}$
 - $U = \hat{U}$ and $V = \Sigma \hat{V}$
 - Too costly in practice

- In PASTIX, rank is decided through an automated way: $||A - UV^T||_F \le \epsilon ||A||_F$

Compression Methods

Partial QR with Column Pivoting (PQRCP)

Main Features

- Column pivoting: column with max 2-norm is the pivot
- $A = UV^T$ compression with column pivoting:

- $AP = Q_{AP}R_{AP}$ is computed, where P is the permutation matrix

-
$$U = Q_{AP}$$
 and $V^T = R_{AP}P^T$

- All the trailing matrix is updated at each iteration

Discussions

- 🙂 Need larger rank than SVD for the same accuracy
- 😕 Not fast enough
- To reduce the cost of pivot selection
 - Randomized method with pivoting

Randomized QR with Column Pivoting (RQRCP)

Main Features

- Create independent and identically distributed Gaussian matrix Ω of size $b \times m,$ where $b \ll m$
- Compute the sample matrix $B = \Omega A$ of size $b \times n$
- Find pivots on B where the row dimension is much smaller than A
 - Less computations
 - Less communication
- Apply this pivoting to A like in PQRCP
- Update whole trailing matrix at each iteration like in PQRCP

Discussions

- 🙂 Similar accuracy to PQRCP
- 🛛 🔀 Not fast enough
- To eliminate the cost of trailing matrix update:

- Truncated randomized method with pivoting

Truncated Randomized QR with Column Pivoting (TRQRCP)

Main Features

- In RQRCP, only the current panel is updated at each iteration
 - Trailing matrix is not needed
- Extra storage: Reflector accumulations
- More efficient on large matrices with small ranks

Discussions

- 🙂 Fastest in sequential
- 🙂 Similar accuracy to previous algorithms
- 😟 Can be improved to give closer ranks to SVD
- Instead of pivoting, apply a reasonable rotation to gather important information to the diagonal blocks
 - Randomized method with rotation

Randomized QR with Rotation (RQRRT)

Main Features

- Similar to RQRCP except:
 - Rotation applied to A
 - Resampling
- In Randomized QR with Column Pivoting (RQRCP):

$$-BP_B = Q_B R_B$$

$$- AP_B = Q_{AP}R_{AP}$$

-
$$U = Q_{AP}$$
 and $V^T = R_{AP}P_B^T$

- In Randomized QR with Rotation (RQRRT):

-
$$B^T = Q_B R_B$$

$$- AQ_B = Q_{AQ}R_{AQ}$$

-
$$U = Q_{AQ}$$
 and $V^T = R_{AQ}Q_B^T$

Discussions

- 🙂 Ranks closest to SVD
- 🧭 Slower and updates whole trailing matrix each iteration

Complexities

- Blue: No change, Green: Reduced cost, Red: More costly
- Matrix size n \times n, block size b, rank k

Methods	Features
SVD: $\mathcal{O}(n^3)$	
PQRCP: $\mathcal{O}(n^2k)$	pivot finding $\mathcal{O}(n^2)$
	trailing matrix update $\mathcal{O}(n^2k)$
PQRCP: $\mathcal{O}(n^2k) \xrightarrow{\text{Randomization}} \text{RQRCP}: \mathcal{O}(n^2k)$	sample matrix generation (beginning) $O(n^2b)$
	pivot finding $\mathcal{O}(nb)$
	update of sample matrix B $\mathcal{O}(\textit{nb}^2)$
	trailing matrix update $\mathcal{O}(n^2k)$
$RQRCP: \mathcal{O}(n^2k) \xrightarrow{Truncation} TRQRCP: \mathcal{O}(nk^2)$	sample matrix generation (beginning) $O(n^2b)$
	pivot finding $\mathcal{O}(nb)$
	update of current panel $\mathcal{O}(nk^2)$
	update of sample matrix B $\mathcal{O}(nb^2)$
$RQRCP \colon \mathcal{O}(n^2k) \xrightarrow{Rotation} RQRRT \colon \mathcal{O}(n^2k)$	resampling (each iteration) $O(n^2b)$
	rotation finding $\mathcal{O}(n^2k)$
	rotation of A $\mathcal{O}(n^2k)$
	trailing matrix update $\mathcal{O}(n^2k)$

- Expected performances (> is better): TQRCP > PQRCP > RQRCP > RQRRT > SVD

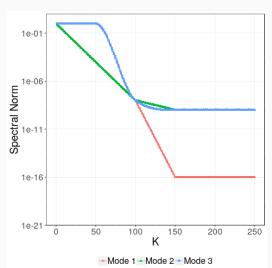
Numerical Results

Test Cases - Singular Values

Spectral Norms

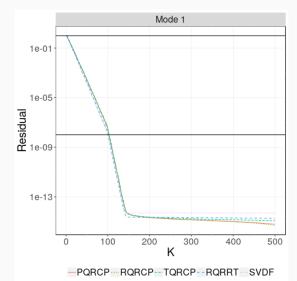
For all Test Cases(Modes):

- Modes are different matrices
- Matrix Size 500
- Rank 100
- Generation Precision 10^{-8}
- $A = UDV^T$
 - D is diagonal matrix with singular values
 - U and V are orthonormal random matrices



Stability - First Test Case Residual Norms

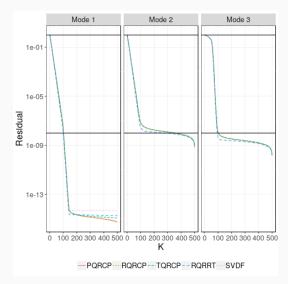
Index vs Error



For all Methods:

- Mode 1
- Matrix is fully factorized without any stopping criterion
- Residual: $\frac{||A U_K V_K^T||_F}{||A||_F}$
- K stands for index values of the matrix

Stability - All Test Cases Residual Norms



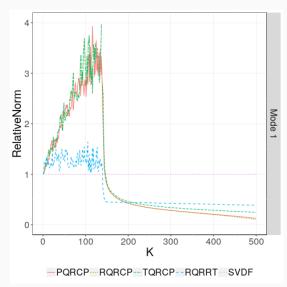
Index vs Error

Stability - First Test Case Relative Residual Norms

Index vs Relative Error

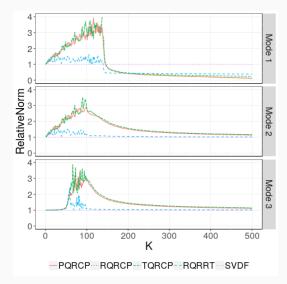
For all Methods:

- Matrix is fully factorized without any stopping criterion
- Relative Norm: <u>Residual</u> <u>Residual</u>^{SVDF}
- K stands for index values of the matrix



Stability - All Test Cases Relative Residual Norms

Index vs Relative Error

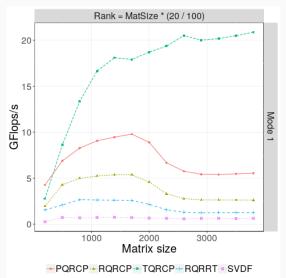


Performance - First Test Case Gflops

Matrix Size vs GFlops

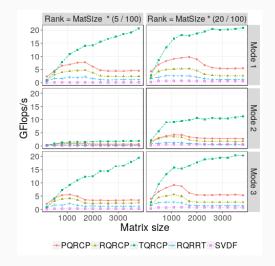
For all Methods:

- Mode 1
- Rank = Matrix_size * $\frac{20}{100}$
- Different matrix sizes are checked
- Compression Precision 10^{-8}
- $GFlops = \frac{min(GFlops)}{t}$
- Threshold is applied



Performance - All Test Cases Gflops

Matrix Size vs GFlops



- Application in the parallel framework of PASTIX with real, larger and tricky matrices
 - Why PQRCP has more performance than RQRCP?
 - TQRCP has the best performance for larger matrices with lower ranks but is not suitable for parallelism
 - RQRRT has the worst QR performance but is promising for parallel environment

- Duersch, J. A.; Gu, M. (2017). "Randomized QR with Column Pivoting".
- Xiao, J.; Gu, M.; Langou, J. (2017). "Fast Parallel Randomized QR with Column Pivoting Algorithms for Reliable Low-rank Matrix Approximations".

Martinsson, P. G. (2015). "Blocked Rank-revealing QR Factorizations: how randomized sampling can be used to avoid single-vector pivoting".

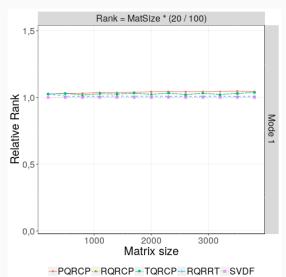
THANK YOU!

Compression Ranks - First Test Case Relative Rank

Matrix Size vs Relative Rank

For all Methods:

- Mode 1
- Rank = Matrix_size * ²⁰/₁₀₀
- Different matrix sizes are checked
- Compression Precision 10^{-8}
- RelativeRank = <u>comp_rank</u> <u>comp_rank^SVDF</u>
- Threshold is applied



Compression Ranks - All Test Cases Relative Rank

