Randomized Algorithms for Computing Full Matrix Factorizations

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Background: Randomized methods such as the "randomized SVD (RSVD)" have proven effective at computing low rank approximations to matrices.

Topic of this talk: How to use methods based on randomized projections to efficiently compute *full* factorizations. Say you want *all* of the eigenvalues, or that the effective rank is not that much smaller than the matrix dimensions (say 10% or 50%).

Themes:

- Use randomization to reduce *communication* rather than flops.
- Quest for algorithms that spend most flops in matrix-matrix multiplications.
- Communication constrained environments:
 - Distributed memory computing.
 - Matrices stored "out-of-core" (say on a hard drive or an SSD).
 - GPU computing.

Outline:

- Review of randomized SVD.
- A randomized method for computing a UTV decomposition. (The UTV decomposition is a relaxation of a singular value decomposition.)
- A randomized method for computing a column pivoted QR decomposition.

Background/review: Randomized singular value decomposition (RSVD)

Problem: Given an $m \times n$ matrix **A**, and a target rank *k*, where $k \ll \min(m, n)$, we seek to compute an approximate partial singular value decomposition:

 $\mathbf{A} \approx \mathbf{U} \quad \mathbf{D} \quad \mathbf{V}^*,$ $m \times n \quad m \times k \ k \times k \ k \times n$

with **U** and **V** having orthonormal columns, and **D** diagonal.

Solution: Pick an over-sampling parameter p, say p = 5. Then proceed as follows:

1. Draw an $n \times (k + p)$ Gaussian random matrix **R**.R = randn(n,k+p)2. Form the $m \times (k + p)$ sample matrix $\mathbf{Y} = \mathbf{A} \mathbf{R}$.Y = A * R3. Form an $m \times (k + p)$ orthonormal matrix \mathbf{Q} s. t. col(\mathbf{Y}) = col(\mathbf{Q}).[Q, ~] = qr(Y)4. Form the $(k + p) \times n$ matrix $\mathbf{B} = \mathbf{Q}^* \mathbf{A}$. $B = Q^* * A$ 5. Compute the SVD of **B** (small!): $\mathbf{B} = \hat{\mathbf{U}} \mathbf{D} \mathbf{V}^*$.[Uhat, Sigma, V] = svd(B, 'econ')6. Form the matrix $\mathbf{U} = \mathbf{Q} \hat{\mathbf{U}}$.U = Q * Uhat

7. Optional: Truncate the last *p* terms in the computed factors.

Background/review: Randomized singular value decomposition (RSVD)

Input:An $m \times n$ matrix **A**, a target rank k, and an over-sampling parameter p (say p = 5).Output:Rank-(k + p) factors **U**, **D**, and **V** in an approximate SVD $\mathbf{A} \approx \mathbf{UDV}^*$.(1)Draw an $n \times (k + p)$ random matrix **R**.(2)Form the $m \times (k + p)$ sample matrix $\mathbf{Y} = \mathbf{AR}$.(3)Compute an ON matrix **Q** s.t. $\mathbf{Y} = \mathbf{QQ}^*\mathbf{Y}$.(4)Form $\mathbf{U} = \mathbf{Q}\hat{\mathbf{U}}$.

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- Often faster than alternative algorithms for low-rank approximation (CPQR, Krylov, ...) on traditional CPU based platforms.
- Order of magnitude acceleration for data stored *out-of-core*.
- Single pass algorithms have been developed for *streaming environments*.
- Consider the problem of computing the dominant k eigenvectors/eigenvalues of a dense matrix of size $m \times n$. Reduction in complexity from O(mnk) to $O(mn\log k)$.
- Highly efficient for GPU computing, or mobile computing (phones, etc).
- Well understood mathematically detailed performance analysis.

Question: Can these ideas be applied for a *full* rank factorization?

Accelerate algorithms for FULL factorizations of matrices

Starting point (Demmel, Dumitriu, Holtz, 2007): Let A be an $n \times n$ matrix. We seek a rank-revealing UTV factorization $A = UTV^*$, with U, V unitary, and T triangular.

Proceed as follows:

- Draw an $n \times n$ Gaussian matrix **G** and orthonormalize its columns $[\mathbf{V}, \sim] = qr(\mathbf{G})$.
- Form a QR factorization of AV so that AV = UT.

Then $\mathbf{A} = \mathbf{UTV}^*$ is provably "rank-revealing." But in a very weak sense.

Improved Demmel UTV (with power iteration): Same set-up.

- Draw an $n \times n$ Gaussian matrix **G** and compute $\mathbf{Y} = (\mathbf{A}^* \mathbf{A})^q \mathbf{G}$ for q = 1 or 2.
- Orthonormalize the columns of **Y** so that $[\mathbf{V}, \sim] = qr(\mathbf{Y})$.
- Form a QR factorization of AV so that AV = UT.

Then $A = UTV^*$ is "rank-revealing." Very good for q = 1. Excellent for q = 2.

These algorithms require a huge number of flops!

But much faster in practice than, say, CPQR.

Key fact: The matrix-matrix multiply can be done *very* rapidly in many environments GPU, distributed memory, fast algorithms, Strassen, etc.

Numerical results for the "Demmel URV" factorization

There are many different ways to measure the quality of a rank-revealing factorization. Let us describe one common measure: Let **A** be an $n \times n$ matrix factored as

$\bm{\mathsf{A}} = \bm{\mathsf{U}}\bm{\mathsf{T}}\bm{\mathsf{V}}^*$

where **U** and **V** are unitary, and where **T** is upper triangular. Define for $k \in \{1, 2, ..., n - 1\}$ the quantities

$$\nu_{k} = \sigma_{k}(\mathbf{T}(1:k,1:k)),$$

$$\tau_{k+1} = \sigma_{1}(\mathbf{T}((k+1):n,(k+1):n)),$$

where $\sigma_i(\mathbf{X})$ denotes the *j*'th singular value of **X**. One can easily prove that

$$\nu_{k} \leq \sigma_{k}(\mathbf{A}) \leq \tau_{k}.$$

The more tightly that (ν_k, τ_k) constrains the k'th singular value, the better.





Singular values and their estimates



Singular values and their estimates







svds Basic URV (upper) Basic URV (lower) CPQR (upper) 10^{-1} CPQR (lower) URV with q=1 (upper) URV with q=1 (lower) in red •• URV with q=2 (upper) 10⁻² URV with q=2 (lower) ь . 10⁻³ 10⁻⁴ 20 40 60 100 120 140 160 80

Singular values and their estimates

The UTV decomposition: A rank-revealing factorization

Given a dense $m \times n$ matrix **A**, with $m \ge n$, compute a factorization

(1)
$$\mathbf{A} = \mathbf{U} \quad \mathbf{T} \quad \mathbf{V}^*,$$
$$m \times n \quad m \times n \quad n \times n \quad n \times n$$

where **T** is upper triangular, and **U** and **V** are unitary. We want a factorization that is "rank-revealing", in the sense its truncation to a rank-*k* approximation should be of close to optimal accuracy. We also would like for the diagonal entries of **T** to approximate the singular values of **A**.

A rank-revealing factorization has many uses:

- Finding a low-rank approximation to a matrix. (Obviously!)
- Solving ill-conditioned linear systems, or linear regression problems.
- Finding bases for fundamental subspaces.

Basically, when (1) is rank-revealing, it can be used for almost anything that the SVD is recommended for.

Given a dense $m \times n$ matrix **A**, with $m \ge n$, compute a factorization

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 $m \times n$ $m \times n n \times n n \times n$

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The technique proposed drives **A** to upper triangular form via unitary transformations:



Both U_i and V_i are (mostly...) products of *b* Householder reflectors.

Blocking enables high performance. Most flops are spent in matrix-matrix multiplication.

The UTV decomposition: A single blocked step

Consider a single blocked step: We apply unitary matrices **U** and **V** to get

 $\mathbf{T} = \mathbf{U}^* \mathbf{A} \mathbf{V}.$

Let *b* be a block size, and separate out the first *b* rows and columns so that

$$\mathbf{T} = \begin{bmatrix} \mathbf{U}_1^* \\ \mathbf{U}_2^* \end{bmatrix} \mathbf{A} \begin{bmatrix} \mathbf{V}_1 & \mathbf{V}_2 \end{bmatrix} = \begin{bmatrix} \mathbf{T}_{11} & \mathbf{T}_{12} \\ \mathbf{0} & \mathbf{T}_{22} \end{bmatrix}$$

We want the following properties in the transformed matrix **T**:

- T_{11} should hold as *much* mass as possible.
- **T**₁₂ should be tiny.

A *perfect* choice of **U** and **V** would be:

- The columns of U_1 span the space spanned by the first k left singular vectors.
- The columns of V_1 span the space spanned by the first k right singular vectors.

We use randomization to cheaply find a *close to optimal* choice:

$$\mathbf{Y} = (\mathbf{A}^* \mathbf{A})^{\boldsymbol{q}} \mathbf{A}^* \mathbf{G}, \qquad [\mathbf{V}, \sim] = qr(\mathbf{Y}),$$

where **G** is an $m \times b$ Gaussian random matrix, and where $q \in \{0, 1, 2\}$. (Over-sampling can be used as well.)

Given a dense $m \times n$ matrix **A**, with $m \ge n$, compute a factorization

 $\mathbf{A} = \mathbf{U} \quad \mathbf{T} \quad \mathbf{V}^*,$

 $m \times n$ $m \times n n \times n n \times n$

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The technique proposed drives **A** to upper triangular form via unitary transformations:



The **V** matrices are found using the randomized projections. (Basically RSVD.)

The **U** matrices zero out the sub-diagonal elements.

Both **U** and **V** must be represented efficiently as products of Householder reflectors. A full, but small (of size $b \times b$) SVD is used to diagonalize the diagonal blocks. *The super-diagonal elements are very small* — *often of relative size* 10^{-5} *or so!*

```
function [U, T, V] = stepUTV(A, b, q)
function [U, T, V] = randUTV(A, b, q)
                                                  G = randn(size(A, 1), b);
  T = A;
                                                  Y = A' *G;
  U = eye(size(A, 1));
                                                  for i = 1:q
  V = eye(size(A, 2));
                                                    Y = A' * (A * Y);
  for i = 1:ceil(size(A, 2)/b)
                                                  end
    I1 = 1: (b * (i-1));
                                                  [V, ~] = qr(Y);
    I2 = (b \star (i-1) + 1) : size(A, 1);
                                                  [U, D, W] = svd(A*V(:, 1:b));
    J2 = (b \star (i-1) + 1) : size(A, 2);
                                                  T = [D, U' * A * \dots
    if (length(J2) > b)
                                                               V(:, (b+1):end)];
       [UU, TT, VV] = stepUTV(T(I2, J2), b, q);
                                                  V(:,1:b) = V(:,1:b) *W;
    else
                                                return
       [UU, TT, VV] = svd(T(I2, J2));
    end
    U(:, I2) = U(:, I2) * UU;
    V(:, J2) = V(:, J2) * VV;
    T(I2, J2) = TT;
    T(I1, J2) = T(I1, J2) * VV;
  end
return
```

Matlab code for the algorithm randUTV that given an $m \times n$ matrix **A** computes its UTV factorization $\mathbf{A} = \mathbf{UTV}^*$. The input parameters b and q reflect the block size and the number of steps of power iteration, respectively. In actual implementations, all unitary matrices are stored as products of Householder reflectors.



Rank-k approximation errors for the matrix "Fast Decay" of size 4000 × 4000. The block size was b = 100. Left: Absolute errors in spectral norm. The black line (circles) marks the theoretically minimal errors. Right: Relative errors $e_k^{\text{relative}} = 100\% \times \frac{\|\mathbf{A} - \mathbf{A}_k\|}{\|\mathbf{A} - \mathbf{A}_k^{\text{optimal}}\|}$.



Rank-k approximation errors for the matrix "S-shape" of size 4000 × 4000. The block size was b = 100. Left: Absolute errors in spectral norm. The black line (circles) marks the theoretically minimal errors. Right: Relative errors $e_k^{\text{relative}} = 100\% \times \frac{\|\mathbf{A} - \mathbf{A}_k\|}{\|\mathbf{A} - \mathbf{A}_k^{\text{optimal}}\|}$.



Rank-k approximation errors for the matrix "Gap" of size 4000 × 4000. The block size was b = 100. Left: Absolute errors in spectral norm. The black line (circles) marks the theoretically minimal errors. Right: Relative errors $e_k^{\text{relative}} = 100\% \times \frac{\|\mathbf{A} - \mathbf{A}_k\|}{\|\mathbf{A} - \mathbf{A}_k\|}$.



Rank-k approximation errors for the matrix "BIE" of size 4000 × 4000. The block size was b = 100. Left: Absolute errors in spectral norm. The black line (circles) marks the theoretically minimal errors. Right: Relative errors $e_k^{\text{relative}} = 100\% \times \frac{\|\mathbf{A} - \mathbf{A}_k\|}{\|\mathbf{A} - \mathbf{A}_k\|}$.

Numerical experiments illustrating how close the UTV is to the SVD

As a consequence of the fact that the super-diagonal elements of **T** are very small, the diagonal elements of **T** are excellent approximants to the singular values of **A**:

$$\mathbf{T}(j,j) \approx \sigma_j, \qquad j = 1, 2 \ldots, \min(m,n).$$

Question: How good?

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Orthonormal matrices (14 cores)



Performances on a 6 x 16 mesh. Orthonormal matrices are built.





Given an $m \times n$ matrix **A** (with $m \ge n$), we seek a QR factorization

 $\mathbf{A} \quad \mathbf{P} \approx \mathbf{Q} \quad \mathbf{R}$

 $m \times n n \times n \qquad m \times k \ k \times n$

for either k = n (full factorization) or k comparable to min(m, n). As usual, **Q** is orthonormal, **P** is a permutation, and **R** is upper triangular.

Question: Is the CPQR "rank-revealing"? Does it satisfy:

• The truncated factorization is a close to optimal low-rank factorization, so that

 $\|\mathbf{A} - \mathbf{Q}(:, 1:k) \mathbf{R}(1:k,:)\mathbf{P}^*\| = \approx \inf\{\|\mathbf{A} - \mathbf{B}\|: \mathbf{B} \text{ has rank } k\}.$

• $\sigma_j(\mathbf{T}(1:k,1:k)) \approx \sigma_j(\mathbf{A}) \text{ for } j \in \{1,2,\ldots,k\}.$

In practice, it is pretty good; it is often used as a cheap substitute for SVD. There are counter-examples, for which it performs very badly.

Note: There are sophisticated pivoting strategies that improve on how well CPQR reveals numerical rank — seminal work by Gu and Eisenstat (1996). Tricky to implement efficiently.

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The technique proposed is based on a blocked version of classical Householder QR:



$$\textbf{A}_0 = \textbf{A} \qquad \textbf{A}_1 = \textbf{Q}_1^* \textbf{A}_0 \textbf{P}_1 \qquad \textbf{A}_2 = \textbf{Q}_2^* \textbf{A}_1 \textbf{P}_2 \qquad \textbf{A}_3 = \textbf{Q}_3^* \textbf{A}_2 \textbf{P}_3 \qquad \textbf{A}_4 = \textbf{Q}_4^* \textbf{A}_3 \textbf{P}_4$$

Each \mathbf{Q}_j is a product of Householder reflectors. Each \mathbf{P}_j is a permutation matrix computed via randomized sampling.

Randomized Column Pivoted QR. *How to do block pivoting using randomization:*

Let **A** be of size $m \times n$, and let *b* be a block size.



Q is a product of *b* Householder reflectors. **P** is a pivoting matrix that moves *b* "pivot" columns to the leftmost slots. We seek **P** so that the set of chosen columns *has maximal spanning volume*. Draw a Gaussian random matrix **G** of size $b \times m$ and form

 $\mathbf{Y} = \mathbf{G} \quad \mathbf{A}$ $b \times n \quad b \times m \quad m \times n$

The rows of **Y** are random linear combinations of the rows of **A**.

Then compute the pivot matrix P for the first block by executing traditional column pivoting on the small matrix Y:

 $\begin{array}{ccc} \mathbf{Y} & \mathbf{P} &= \mathbf{Q}_{\text{trash}} & \mathbf{R}_{\text{trash}} \\ \mathbf{b} \times \mathbf{n} & \mathbf{n} \times \mathbf{n} & \mathbf{b} \times \mathbf{b} & \mathbf{b} \times \mathbf{n} \end{array}$

References: Martinsson, arxiv, 2015. Martinsson, Quintana-Orti, Heavner, van de Geijn, SISC, 2017. Duersch & Gu, arxiv, 2015. Duersch & Gu, SISC, 2017.

Connection to randomized Interpolatory Decomposition (ID), CUR, etc.

Let **A** be an $m \times n$ matrix of numerical rank k. An *Interpolatory Decomposition (ID)* of **A** takes the form

$$\mathbf{A} \approx \mathbf{C} \mathbf{X}$$

 $m \times n$ $m \times k \ k \times n$

where **C** consists of *k* columns of **A**, and where **X** is a well-conditioned matrix.

Let J_s denote an index vector identifying the "skeleton" columns so that $\mathbf{C} = \mathbf{A}(:, J_s)$.

A randomized algorithm for computing the ID, given an over-sampling parameter *p*:

- Draw a $(k + p) \times m$ Gaussian matrix **G**.
- Form a $(k + p) \times n$ sampling matrix $\mathbf{Y} = \mathbf{GA}$.
- Perform a rank-*k* CPQR on **Y** so that $\mathbf{Y} \approx \mathbf{Y}(:, J_s)\mathbf{X}$.

Then we automatically (and almost magically) get an ID of A:

$$\mathbf{A} \approx \mathbf{A}(:, J_{\mathrm{S}})\mathbf{X}.$$

Can be used to compute a CUR decomposition as well.

Reference: "Randomized algorithms for the low-rank approximation of matrices." E. Liberty, F. Woolfe, P.G. Martinsson, V. Rokhlin, and M. Tygert; PNAS, 2007



Speedup attained by our randomized algorithm HQRRP for computing a full column pivoted QR factorization of an n × n matrix. The speed-up is measured versus LAPACK's faster routine dgeqp3 as implemented in Netlib (left) and Intel's MKL (right). Our implementation was done in C, and was executed on an Intel Xeon E5-2695. Joint work with G. Quintana-Ortí, N. Heavner, and R. van de Geijn. Available at: https://github.com/flame/hqrrp/



For the task of computing low-rank approximations to matrices, the classical choice is between SVD and column pivoted QR (CPQR). SVD is slow, and CPQR is inaccurate:



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The randomized algorithm randUTV combines the best properties of both factorizations. Additionally, randUTV parallelizes better, and allows the computation of partial factorizations (like CPQR, but unlike SVD).

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Future work: Continued development or randCPQR and randUTV. Adapt to different computing architectures (distributed memory, out-of-core, etc). Theory. Exploit information that is currently wasted. Multiple sweeps version. Algorithm-by-blocks.

For the task of computing low-rank approximations to matrices, the classical choice is between SVD and column pivoted QR (CPQR). SVD is slow, and CPQR is inaccurate:



Block Krylov methods: For partial factorizations of sparse matrices, integrate ideas from Krylov methods. Explore design space between the basic RSVD and classical "single-vector" Krylov methods. Recent work by Musco & Musco; Tropp; Gu.

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Software for UTV: https://github.com/flame/randutv Software for CPQR: https://github.com/flame/hqrrp