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Random Orthogonal Matrices in High Performance Computing

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Slides available at https://bit.ly/rom-hpc

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What Is a Random Orthogonal Matrix?

Distributed according to the Haar measure over the group of orthogonal matrices.

- Haar measure provides a uniform distribution over the orthogonal matrices.
- Haar measure is invariant under mult on left and right by orthogonal matrices: if Q is distributed so is UQV for any orthogonal (possibly non-random) U and V.

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These are *not* Haar distributed, where $S = -S^T$:

- random Householder matrix,
- random Cayley transform $(I + S)(I - S)^{-1}$,
- e^S.

Randsvd Matrices

$$A = P\Sigma Q^T \in \mathbb{R}^{m\times n}, \quad P, Q \text{ random orthogonal}$$
$$\Sigma = \mathrm{diag}(\sigma_1, \sigma_2, \dots, \sigma_n), \quad \sigma_1 \ge \sigma_2 \ge \cdots \ge \sigma_n \ge 0.$$

- **Demmel & McKenney (1989)**: LAPACK's test matrix generation suite.
- **H (1991, 1995)**: MATLAB function `randsvd`. Subsequently incorporated into `gallery('randsvd',...)`.
- **H & Zhang (2016)**: Matrix Depot package for Julia.

Generating Q

Method 1 (inefficient).

```
[Q,R] = qr(randn(n));
Q = Q*diag(sign(diag(R)));
```

Method 2 (efficient, product form, no R).
Stewart (1980): Let $x_k \in \mathbb{R}^{n-k+1}$ be normal (0,1).
H_k Householder matrix that reduces x_k to $r_{kk} e_1$.

$$Q = DH_1' H_2' \dots H_{n-1}',$$

where $H_k' = \text{diag}(I_{k-1}, H_k)$, $D = \text{diag}(\text{sign}(r_{kk}))$, $r_{nn} = x_n$.

- In MATLAB, `Q = gallery('qmult',n)`.
- Halves cost of forming a randsvd matrix: $\approx m^3 + n^3$ flops.

Cheaper Randsvd Matrix

Want to compute A in $O(mn)$ flops.

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Want to compute A in $O(mn)$ flops.

- In $A = P\Sigma Q^T$, give up P and Q Haar-distributed, or even random.
- Could use same construction with $k \le \min(m, n)$ Householders.

Cheaper Randsvd Matrix

- Let

$$A = Q\Sigma W^T,$$

where Q has orthonormal cols and W is a random (rectangular) Householder matrix.

- For $m = n$, if only $\kappa_2(A)$ is to be specified, can reduce the cost of formation by setting $\sigma_2 = \cdots = \sigma_{n-1} = 1$.

Properties

- Form in $O(mn)$ flops + cost of Q.
- Little communication required.

M. Fasi and N. J. Higham. **Generating extreme-scale matrices with specified singular values or condition numbers**. MIMS EPrint 2020.8, March 2020.

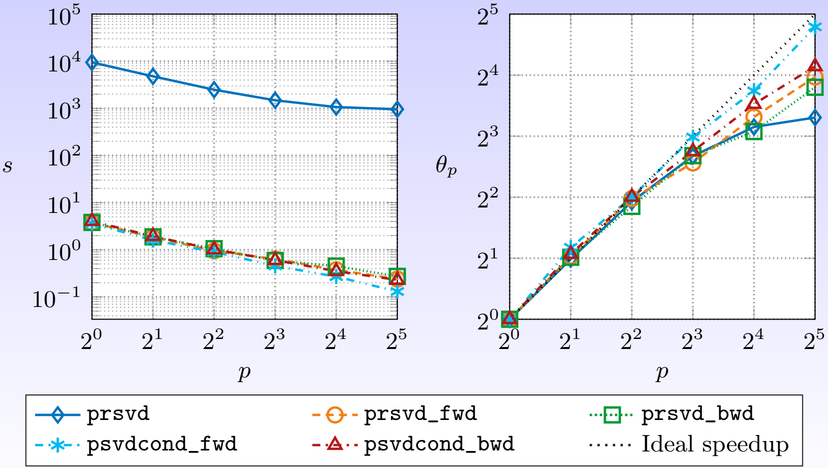
Choice of Q

- Haar distributed *or*
- to reduce communication, $Q = (f(i,j))$, such as

$$q_{ij} = \frac{2}{\sqrt{2n+1}} \sin\left(\frac{2ij\pi}{2n+1}\right).$$

Experiment, $n = 20,000$

- In C using BLACS, PBLAS, ScaLAPACK, Open MPI.
- Nodes have two 16-core Intel Xeon CPUs.
- p processes. Wall clock (left), speedup t_1/t_p (right).



The Growth Factor

Gaussian elimination on $A \in \mathbb{R}^{n \times n}$ produces $A = LU$.

With $A^{(1)} = A$, $A^{(n)} = U$, $A^{(k)} = \left(a_{ij}^{(k)}\right)$ matrix at kth stage of Gaussian elimination,

$$\rho_n(A) = \frac{\max_{i,j,k} |a_{ij}^{(k)}|}{\max_{i,j} |a_{ij}|} \geq 1.$$

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Theorem (Wilkinson, 1961)

GE produces a computed solution $\widehat{x}$ to $Ax = b$ satisfying

$$(A + \Delta A)\widehat{x} = b, \qquad \|\Delta A\|_\infty \leq p(n)\rho_n u \|A\|_\infty,$$

where u is unit roundoff and p a low degree polynomial.

What We Know About the Growth Factor

- Without pivoting, ρ_n can arbitrarily large.
- With **partial pivoting**, $\rho_n \le 2^{n-1}$, attained for

$$A_4 = \begin{bmatrix} 1 & 0 & 0 & 1 \\ -1 & 1 & 0 & 1 \\ -1 & -1 & 1 & 1 \\ -1 & -1 & -1 & 1 \end{bmatrix}.$$

- **Wright (1993)** and **Foster (1994)** found applications where partial pivoting suffers exponential growth.
- **Higham & Higham (1989)** found orthogonal matrices with $\rho_n \gtrsim n/2$ for *any* pivoting strategy.
- In practice, ρ_n is **almost always small** for partial pivoting. *Open problem to explain why!*

MATLAB Function

```
function g = gf(A)
%GF     Approximate growth factor.
%   g = GF(A) is an approximation to the
%   growth factor for LU factorization
%   with partial pivoting.
[~,U] = lu(A);
g = max(abs(U),[],'all')/max(abs(A),[],'all');
```

- This is a lower bound on $\rho_n(A)$.
- Can get exact growth factor using `gep.m` from **Matrix Computation Toolbox**.

```
>> rng(1); gf(randn(10))
ans =
   1.5088e+00
>> gf(randn(100))
ans =
   4.4874e+00
>> gf(randn(1000))
ans =
   1.5997e+01
>> gf(randn(10000))
ans =
   5.0505e+01
>> gf(gallery('randsvd',1000,1e8,2,[],[],1))
ans =
   7.5329e+01
```

Does $O(n)$ Growth Matter?

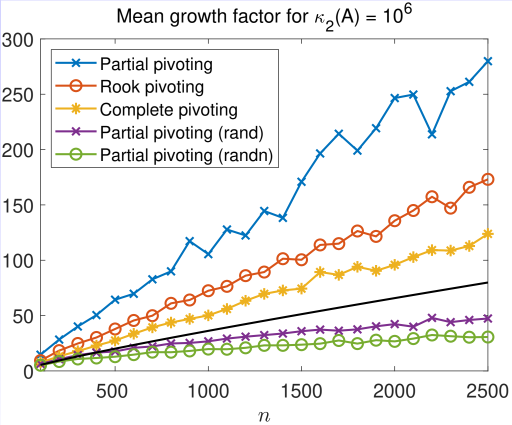
- $n = 10^7$ for today's largest dense $Ax = b$
$\Rightarrow$ problems in single precision.

- For IEEE half precision and $\max_{i,j} |a_{ij}| = 1$, linear growth can cause overflow for $n = 7 \times 10^4$.
(That's how these matrices were spotted.)

D. J. Higham, N. J. Higham, and S. Pranesh. **Random matrices generating large growth in LU factorization with pivoting**. MIMS EPrint 2020.13, May 2020.

Randsvd Matrices (Mode 2)

$$A = P\Sigma Q^T \in \mathbb{R}^{n\times n}, \quad P^TP = Q^TQ = I,$$
$$\Sigma = \mathrm{diag}(1,\dots,1,\sigma_n), \quad 1 \ge \sigma_n \ge 0.$$



Growth Factor Lower Bound

Theorem (H & H, 1989)

Let $A \in \mathbb{C}^{n\times n}$ be nonsingular,

$$\alpha = \max_{i,j} |a_{ij}|, \quad \beta = \max_{i,j} \left|\left(A^{-1}\right)_{ij}\right|, \quad \theta = (\alpha\beta)^{-1}.$$

Then $\theta \le n$, and for any permutation matrices Π_r and Π_c such that $\Pi_r A \Pi_c$ has an LU factorization, the growth factor for GE without pivoting on $\Pi_r A \Pi_c$ satisfies

$$\rho_n(A) \ge \theta.$$

Growth for Random Orthogonal Matrices

Randsvd with $\sigma_n = 1$ gives $A = PQ^T$: **random orthogonal matrix from Haar distribution**.

Jiang (2005) shows that

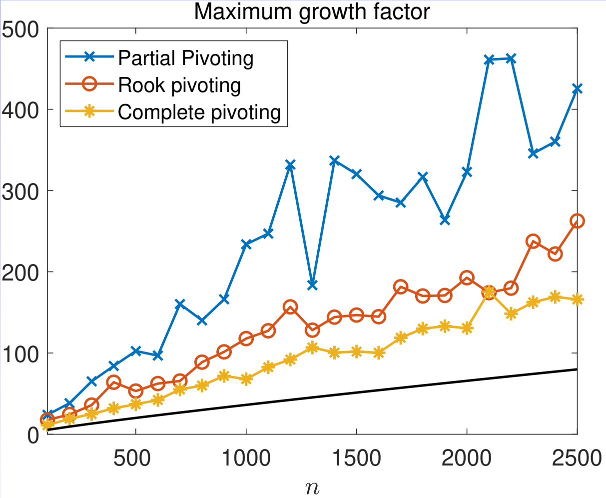
$$\Pr\left(\max_{i,j} |a_{ij}| > 2\sqrt{\frac{\log(n)}{n}}(1+\epsilon)\right) \to 0$$

as $n \to \infty$ for any $\epsilon > 0$. Since $A^{-1} = A^T$, can take $\alpha = \beta = 2\sqrt{\log(n)/n}$ in the theorem and conclude

$$\rho_n(A) \gtrsim \frac{n}{4 \log n}$$

for large n with high probability for *any* pivoting strategy.

Growth Factors for Random Orthogonal



Proof of Large Growth for Randsvd

- The randsvd matrix is

$$A = PQ^T + (\sigma_n - 1)p_n q_n^T,$$

  where p_n and q_n are the last columns of P and Q.

- If W is orthogonal and has large growth then a rank-1 perturbation of norm at most 1 *tends to preserve the large growth*.
- **Not particular** to W being Haar distributed.
- One approach is via **Sherman–Morrison formula**.

Direct Approach

Let W be orthogonal and

$$A = W + xy^T.$$

The U factor of W is given explicitly by

$$u_{ij} = \frac{\det\big(W(1\colon i, [1\colon i-1,\ j])\big)}{\det(W_{i-1})}, \qquad i \le j,$$

where $W_j = W(1\colon j, 1\colon j)$. Find $\widetilde{U}$ factor of A satisfies

$$\frac{\widetilde{u}_{ij}}{u_{ij}} = \frac{1 + y([1\colon i-1,\ j])^T\ W(1\colon i, [1\colon i-1,\ j])^{-1}\ x(1\colon i)}{1 + y(1\colon i-1)^T\ W_{i-1}^{-1}\ x(1\colon i-1)}.$$

Singular Values of Submatrix of W

Lemma

Let $W \in \mathbb{R}^{n\times n}$ be orthogonal and

$$\begin{array}{c c} & \begin{array}{cc} n-k & k \end{array} \\ \begin{array}{c} n-k \\ k \end{array} & \begin{bmatrix} W_{11} & W_{12} \\ W_{12} & W_{22} \end{bmatrix}, \end{array}$$

where $k < n/2$. Then W_{11} has at least $n-2k$ singular values equal to 1 and the remaining k singular values are bounded above by 1.

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Proof. Use the CS decomposition. □

Iterative Refinement

For $Ax = b$, with precisions **low**, **medium**, **high**.

- Factorize $A = LU$ in **low**.
- Solve $Ax = b$ in **low**.
- Repeat
  - $r = b - Ax$ in **high**.
  - Solve $Ad = r$ in **medium** using LU factors.
    or
  - Solve $U^{-1}L^{-1}Ad = U^{-1}L^{-1}r$ by GMRES in **medium**.
  - $x \leftarrow x + d$ in **medium**.

Large growth does not inhibit convergence of IR.

Summary

New class of **random**, dense $A \in \mathbb{R}^{n\times n}$ (*randsvd mode* 2) for which

- $\rho_n \gtrsim n/(4 \log n)$ for large n with **any form of pivoting**,
- $\kappa_2(A)$ can be **arbitrarily chosen**.

Have been part of MATLAB **gallery** for many years but their growth properties had not been recognized.

- New algorithm forms "randsvd-like" matrices at cost linear in # matrix elements, with little communication.
- Beware mode 2!

Slides available at `https://bit.ly/rom-hpc`

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