Reliability issues in SVD and PSVD software

A case study

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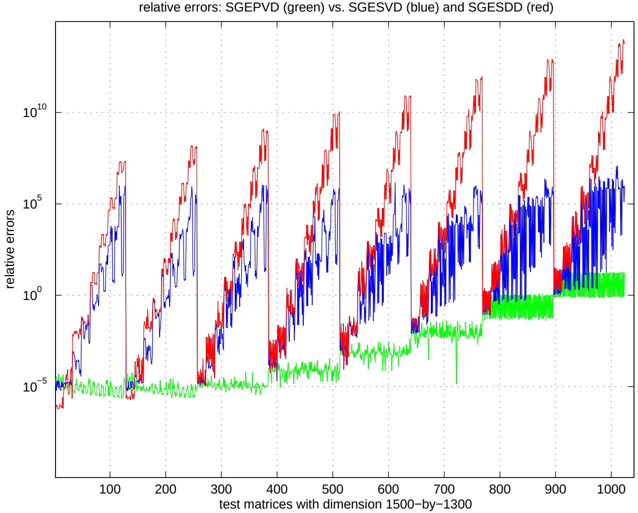
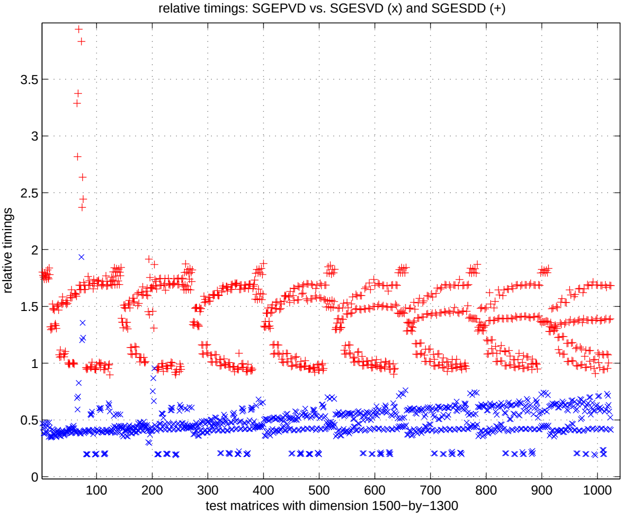
Outline

Accuracy: $\max_i \frac{|\tilde{\sigma}_i - \sigma_i|}{\sigma_i}$



Relative error: $A = BD$: Jacobi, SGESVD, SGESDD

Improved efficiency



Timings: Jacobi/SGESVD, Jacobi/SGESDD

QRCP as preconditioner

$$AP = Q\begin{pmatrix} R \\ 0 \end{pmatrix}; \quad A = \begin{pmatrix} \blacksquare \\ \blacksquare \\ \blacksquare \end{pmatrix}, R = \begin{pmatrix} \blacksquare \end{pmatrix}$$

$\mathrm{SVD}(R) \hookrightarrow \mathrm{SVD}(A)$, $\mathrm{SVD}(R^T) \hookrightarrow \mathrm{SVD}(A)$

- $P^T A^T A P = R^T R$
  - $X = R$, diagonalize $X^T X = R^T R$;
  - $X \underbrace{J_1 J_2 \cdots J_\infty}_{V_x} = U_x \Sigma \Longrightarrow R \equiv X = U_x \Sigma V_x^T$
- $AA^T = Q\begin{pmatrix} RR^T & 0 \\ 0 & 0 \end{pmatrix} Q^T$
  - $X = R^T$, diagonalize $X^T X = RR^T$;
  - $X \underbrace{J_1 J_2 \cdots J_\infty}_{V_x} = U_x \Sigma \Longrightarrow R \equiv X^T = V_x \Sigma U_x^T$

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★ $$|R_{ii}| \geq \sqrt{\sum_{k=i}^{j} |R_{kj}|^2}, \quad \text{for all } 1 \leq i \leq j \leq n.$$

$$|R_{11}| \geq |R_{22}| \geq \cdots \geq |R_{nn}|$$

★ may not be rank revealing

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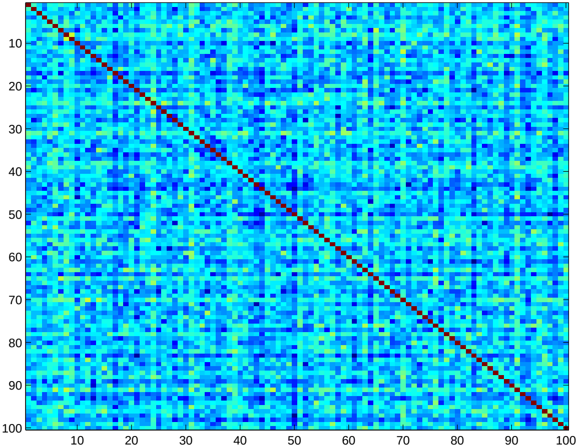

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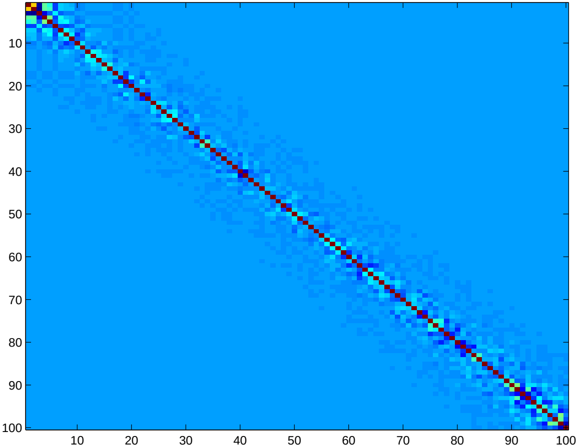

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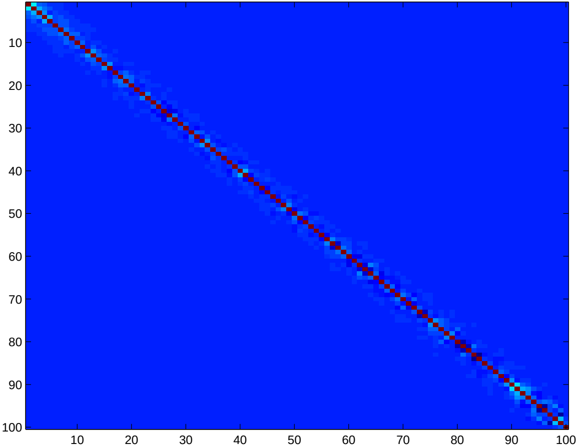
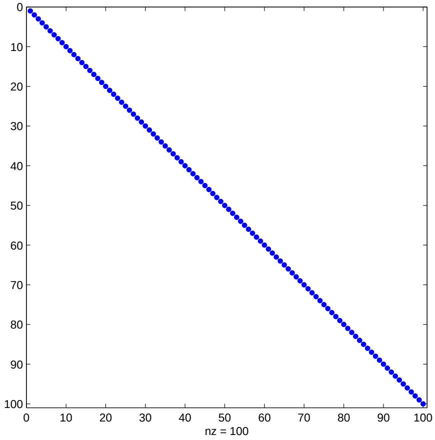


$$R^T P_1 = Q_1 R_1;\ R^T R = Q_1 R_1 R_1^T Q_1^T$$

QR as preconditioner



spy(P1)

Jacobi ++

- $(\Pi A)P = Q\begin{pmatrix} R \\ 0 \end{pmatrix}$; $\rho = \mathrm{rank}(R)$ $(A = D_1 B D_2)$
  - $R(1:\rho, 1:n)^T = Q_1\begin{pmatrix} R_1 \\ 0 \end{pmatrix}$;
  - $X = R_1^T = \begin{pmatrix} \blacksquare & 0 \\ \blacksquare & \blacksquare \end{pmatrix}$; $X^T X - \xi I$ quasi–definite
    - $X_\infty \equiv U_x \Sigma = X \underbrace{\langle J_1 J_2 \cdots J_\infty \rangle}_{V_x}$
    - $V_x = R_1^{-T}(X_\infty)$
- $U = \Pi^T Q\begin{pmatrix} U_x & 0 \\ 0 & I_{m-\rho} \end{pmatrix}$; $V = PQ_1\begin{pmatrix} V_x & 0 \\ 0 & I_{n-\rho} \end{pmatrix}$
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Testing the new software

- Our tests are rigorous
  - full range, $\sigma_i \in$(small, BIG)
  - two levels of accuracy
    - $|\tilde{\sigma}_i - \sigma_i| \leq K \cdot \epsilon \cdot \|A\|_2$ for all i
    - $|\tilde{\sigma}_i - \sigma_i| \leq C \cdot \epsilon \cdot \sigma_i$ for all i
  - theoretical bounds attained
  - no surprises
- All passed.
- Then we started looking for trouble. That is our job.

And we found trouble. We got surprised.

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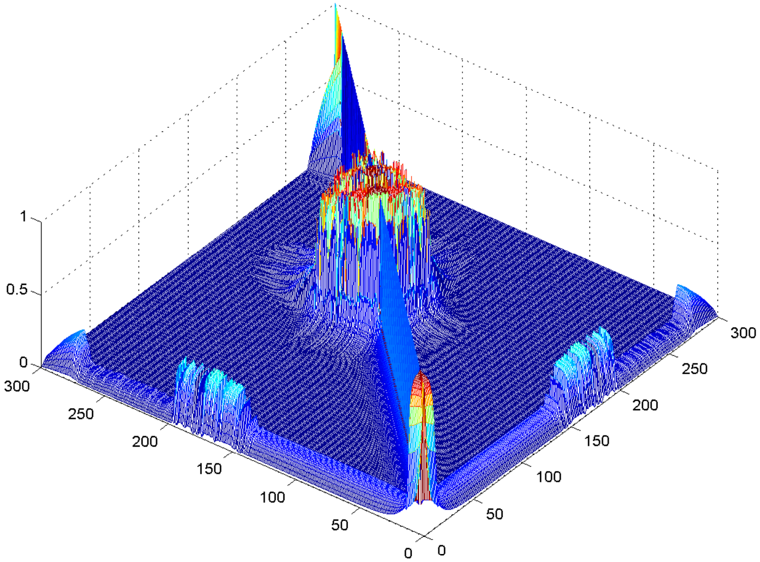
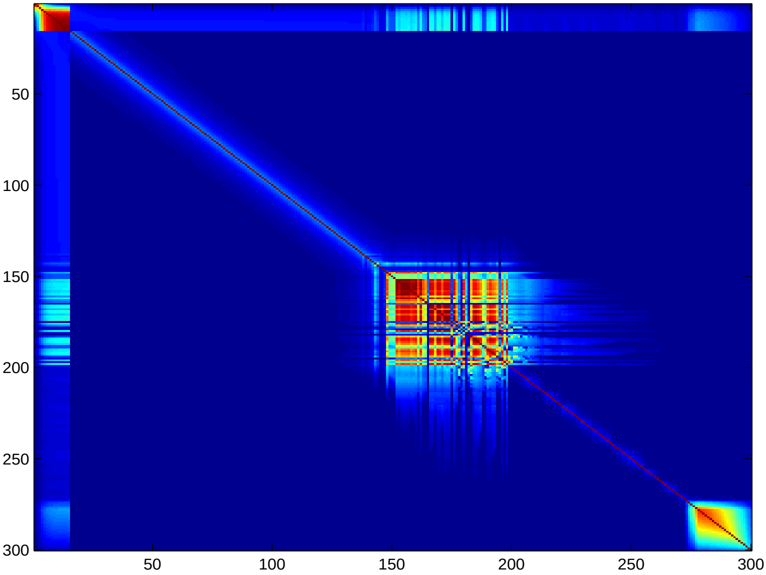


$\mathfrak{K} = Kahan(n, c)$; $A = \mathfrak{K} + \mathfrak{K}^T$. RR^T. *The ill–conditioned "tower" is a result of wrong pivot choices.*



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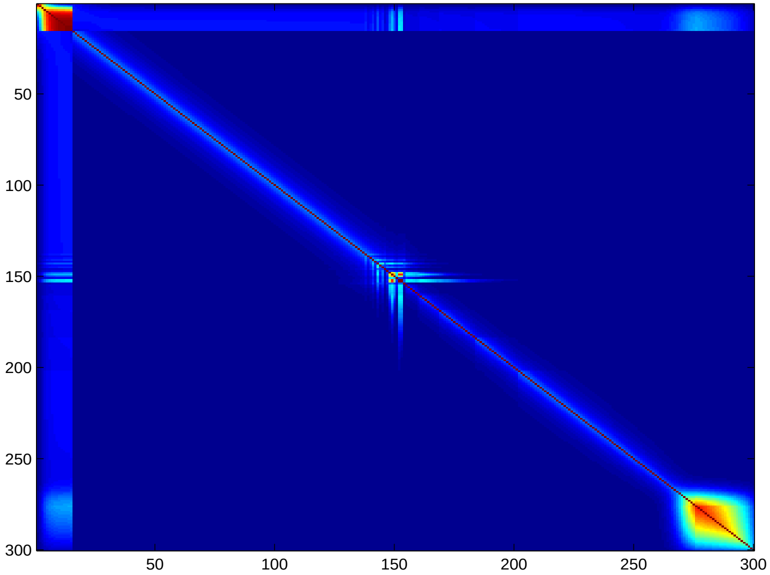

$$\mathfrak{K} = Kahan(n, c\cdot(1+\epsilon));\ A = \mathfrak{K} + \mathfrak{K}^T.\ RR^T.$$

Businger–Golub pivoting

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$$|R_{11}| \geq |R_{22}| \geq \cdots \geq |R_{nn}|$$

★ may not be rank revealing but it must be guaranteed by the software (xGEQPF, xGEQP3)

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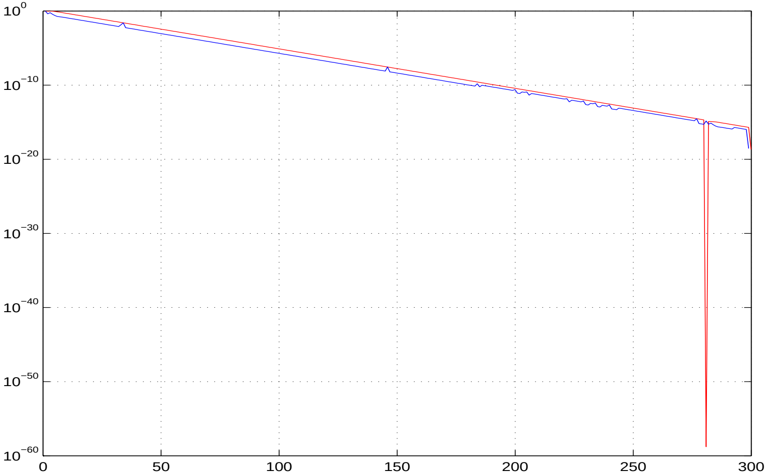
Examples of failure of ★



$|R_{ii}|$, $\max_{j\geq i} \sqrt{\sum_{k=i}^{j} |R_{kj}|^2}$

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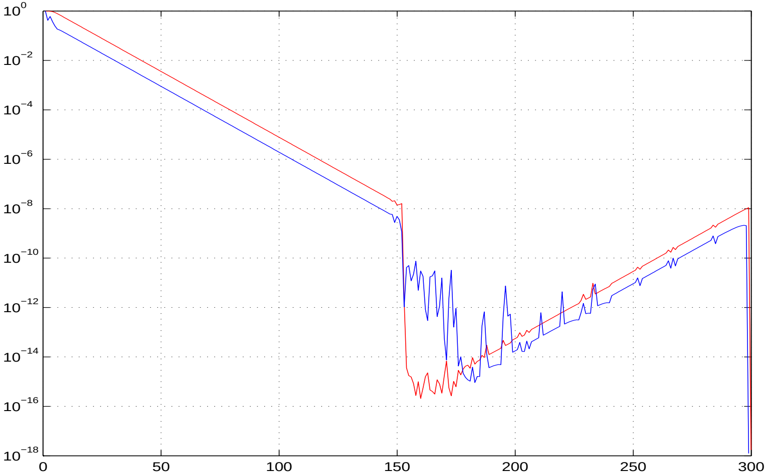

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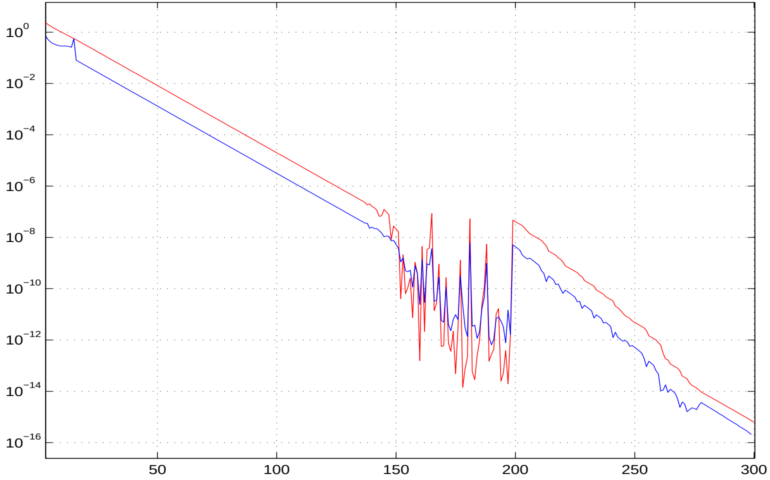

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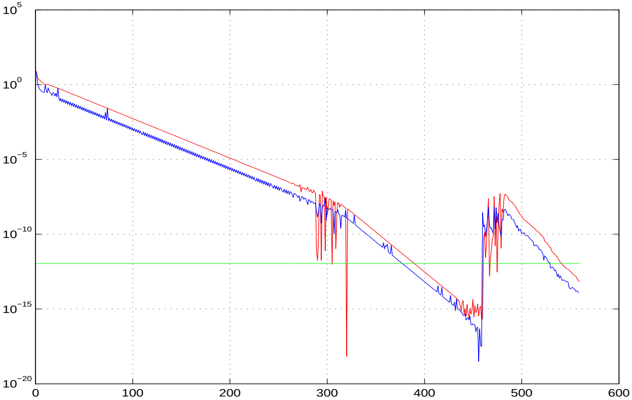
Consequences

$\|Ax - d\|_2 \rightarrow \min; x = A \backslash d$

`Warning: Rank deficient, rank = 304 tol = 1.0994e-012.`



`rank(`A`,1.0994e-12)` returns 466

Consequences

Any routine based on xQRDC (LINPACK) or xGEQPF, xGEQP3 (LAPACK) can catastrophically fail.

- xGEQPX (TOMS ♯ 782, rank revealing QRF)
- xGELSX and xGELSY in LAPACK ($\|Ax - b\|_2 \rightarrow \min$)
- xGGSVP in LAPACK (GSVD of (A, B))

$$U^T A Q = \begin{pmatrix} 0 & A_{12} & A_{13} \\ 0 & 0 & A_{23} \\ 0 & 0 & 0 \end{pmatrix}, \quad V^T B Q = \begin{pmatrix} 0 & 0 & B_{13} \\ 0 & 0 & 0 \end{pmatrix}.$$

- ... and many others ... long list. Need a new xGEQP3.

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L(IN+A)PACK update

$$A^{(k)}\Pi_k = \begin{pmatrix} \cdot & \cdot & \odot & \cdot & \oplus & \cdot \\ & \cdot & \odot & \cdot & \oplus & \cdot \\ & & \blacksquare & \circledast & \circledast & \circledast \\ & & \circledcirc & * & * & * \\ & & \circledcirc & * & * & * \\ & & \circledcirc & * & * & * \end{pmatrix}, \quad \mathbf{a}_j^{(k)} = \begin{pmatrix} \oplus \\ \oplus \\ \circledast \\ * \\ * \\ * \end{pmatrix} \equiv \begin{pmatrix} \mathbf{x}_j^{(k)} \\ \mathbf{z}_j^{(k)} \end{pmatrix} \tag{1}$$

$$\mathrm{H}_k \mathbf{z}_k^{(k)} = \begin{pmatrix} R_{kk} \\ 0 \end{pmatrix}, \begin{pmatrix} \beta_j^{(k+1)} \\ \mathbf{z}_j^{(k+1)} \end{pmatrix}, \quad \omega_j^{(k)} = \|\mathbf{z}_j^{(k)}\| = \mathrm{H}_k \mathbf{z}_j^{(k)}. \tag{2}$$

$$\|\mathbf{z}_j^{(k+1)}\| \equiv \omega_j^{(k+1)} = \sqrt{(\omega_j^{(k)})^2 - (\beta_j^{(k+1)})^2},$$ provided that

$$\mathit{computed}\left(\left(1 - \left(\frac{\tilde{\beta}_j^{(k+1)}}{\tilde{\omega}_j^{(k)}}\right)^2\right) \cdot \left(\frac{\tilde{\omega}_j^{(k)}}{\tilde{\nu}_j}\right)^2\right) > tol, \quad tol \approx 20\varepsilon,$$

L(IN+A)PACK update

$$A^{(k)}\Pi_k = \begin{pmatrix} \cdot & \cdot & \odot & \cdot & \oplus & \cdot \\ & \cdot & \odot & \cdot & \oplus & \cdot \\ & & \blacksquare & \circledast & \circledast & \circledast \\ & & \circledcirc & * & * & * \\ & & \circledcirc & * & * & * \\ & & \circledcirc & * & * & * \end{pmatrix}, \quad \mathbf{a}_j^{(k)} = \begin{pmatrix} \oplus \\ \oplus \\ \circledast \\ * \\ * \\ * \end{pmatrix} \equiv \begin{pmatrix} \mathbf{x}_j^{(k)} \\ \mathbf{z}_j^{(k)} \end{pmatrix} \quad (1)$$

$$\mathrm{H}_k \mathbf{z}_k^{(k)} = \begin{pmatrix} R_{kk} \\ 0 \end{pmatrix}, \begin{pmatrix} \beta_j^{(k+1)} \\ \mathbf{z}_j^{(k+1)} \end{pmatrix}, \quad \omega_j^{(k)} = \|\mathbf{z}_j^{(k)}\| = \mathrm{H}_k \mathbf{z}_j^{(k)}. \quad (2)$$

$$\|\mathbf{z}_j^{(k+1)}\| \equiv \omega_j^{(k+1)} = \sqrt{(\omega_j^{(k)})^2 - (\beta_j^{(k+1)})^2},$$ provided that

$$\textit{computed}\left(\left(1 - \left(\frac{\tilde{\beta}_j^{(k+1)}}{\tilde{\omega}_j^{(k)}}\right)^2\right) \cdot \left(\frac{\tilde{\omega}_j^{(k)}}{\tilde{\nu}_j}\right)^2 \right) > tol, \quad tol \approx 20\varepsilon,$$

L(IN+A)PACK update

```
      DO 30 J = I+1, N
         IF ( WORK( J ).NE.ZERO ) THEN
            TEMP = ONE - ( ABS( A( I, J ) ) / WORK( J ) )**2
            TEMP = MAX( TEMP, ZERO )
            TEMP2 = ONE + 0.05*TEMP*( WORK( J ) / WORK( N+J ) )**2
            WRITE(*,*) TEMP2
            IF( TEMP2.EQ.ONE ) THEN
               IF( M-I.GT.0 ) THEN
                  WORK( J ) = SNRM2( M-I, A( I+1, J ), 1 )
                  WORK( N+J ) = WORK( J )
               ELSE
                  WORK( J ) = ZERO
                  WORK( N+J ) = ZERO
               END IF
            ELSE
               WORK( J ) = WORK( J )*SQRT( TEMP )
            END IF
         END IF
30    CONTINUE
```

g77 -c -O -ffloat-store

Critical part in the column norm update. (For the full source see http://www.netlib.org/lapack/single/sgeqpf.f)

NEW update

$$A^{(k)}\Pi_k = \begin{pmatrix} \cdot & \cdot & \odot & \cdot & \oplus & \cdot \\ & \cdot & \odot & \cdot & \oplus & \cdot \\ & & \blacksquare & \circledast & \circledast & \circledast \\ & & \circledcirc & \ast & \ast & \ast \\ & & \circledcirc & \ast & \ast & \ast \\ & & \circledcirc & \ast & \ast & \ast \end{pmatrix}, \quad \mathbf{a}_j^{(k)} = \begin{pmatrix} \oplus \\ \oplus \\ \circledast \\ \ast \\ \ast \\ \ast \end{pmatrix} \equiv \begin{pmatrix} \mathbf{x}_j^{(k)} \\ \mathbf{z}_j^{(k)} \end{pmatrix} \tag{3}$$

$$\mathrm{H}_k \mathbf{z}_k^{(k)} = \begin{pmatrix} R_{kk} \\ 0 \end{pmatrix}, \begin{pmatrix} \beta_j^{(k+1)} \\ \mathbf{z}_j^{(k+1)} \end{pmatrix}, \quad \omega_j^{(k)} = \|\mathbf{z}_j^{(k)}\| = \mathrm{H}_k \mathbf{z}_j^{(k)}. \tag{4}$$

$$\|\mathbf{a}_j^{(k)}\| = \alpha_j^{(k)} = \alpha_j^{(0)}; \quad \xi_j^{(k+1)} = \sqrt{(\xi_j^{(k)})^2 + (\beta_j^{(k+1)})^2}$$

$$\|\mathbf{z}_j^{(k+1)}\| \equiv \omega_j^{(k+1)} = \sqrt{(\alpha_j^{(0)})^2 - (\xi_j^{(k+1)})^2}$$

NEW update

Z.D. and Z. Bujanović, Zagreb 2006
New code xGEQP3Z tested.

- Provably delivers Businger–Golub structured R (up to roundoff)
- Same efficiency as xGEQP3 (up to $\pm\ 3 - 4$ %)
- Makes our Jacobi SVD code more robust
- Makes many other solvers more robust and can prevent catastrophes in mission critical applications
- Recommended as replacement for xGEQP3 from LAPACK

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PSVD

$A = BC^T = U\Sigma V^T$, B, C full column rank

$$BC^T = \begin{pmatrix} \blacksquare & \blacksquare & \blacksquare \\ \blacksquare & \blacksquare & \blacksquare \\ \blacksquare & \blacksquare & \blacksquare \\ \blacksquare & \blacksquare & \blacksquare \end{pmatrix} \begin{pmatrix} \blacksquare & \blacksquare & \blacksquare & \blacksquare \\ \blacksquare & \blacksquare & \blacksquare & \blacksquare \\ \blacksquare & \blacksquare & \blacksquare & \blacksquare \end{pmatrix}$$

- A=yxGEMM(B,C^T) fastesssst matrix multiply
- CALL yxGESDD(A) fastesssst SVD
- $\begin{pmatrix} 1 & \epsilon \\ -1 & \epsilon \end{pmatrix} \begin{pmatrix} 2 & 2 \\ 2 & 1 \end{pmatrix} = \begin{pmatrix} 2+2\epsilon & 2+\epsilon \\ -2+2\epsilon & -2+\epsilon \end{pmatrix} \approx \begin{pmatrix} 2 & 2 \\ -2 & -2 \end{pmatrix}$
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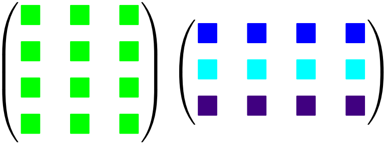
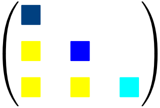
PSVD

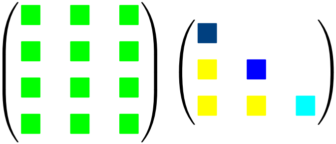
Z.D. 1998., now improved

$BC^T =$ 

- $CP = Q \begin{pmatrix} R \\ 0 \end{pmatrix}$; $BC^T = (BP)\begin{pmatrix} R^T & 0 \end{pmatrix} Q^T$;
- $A = (BP)R^T$; $R^T =$ 
- $[U, \Sigma, V_1]$=SVD(A); $V = Q \begin{pmatrix} V_1 & 0 \\ 0 & I_{n-p} \end{pmatrix}$

And what about BPR^T?

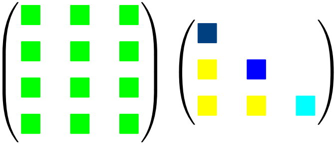
$BPT^T \equiv$



Consider $\begin{pmatrix} a_1 & a_2 & a_3 \end{pmatrix} = \begin{pmatrix} b_1 & b_2 & b_3 \end{pmatrix} \begin{pmatrix} \ell_{11} & 0 & 0 \\ \ell_{21} & \ell_{22} & 0 \\ \ell_{31} & \ell_{32} & \ell_{33} \end{pmatrix}$

$$\begin{aligned}
\tilde{a}_3 &= (b_3 + \delta b_3)\ell_{33} \\
\tilde{a}_2 &= (b_2 + \delta_2 b_2)\ell_{22} + (b_3 + \delta_2 b_3)\ell_{32} \\
&= (b_2 + \delta_2 b_2)\ell_{22} + (b_3 + \delta b_3 - \delta b_3 + \delta_2 b_3) \\
&= (b_2 + \delta_2 b_2 + (\delta_2 b_3 - \delta b_3)\frac{\ell_{32}}{\ell_{22}})\ell_{22} + (b_3 + \delta b_3)\ell_{33} \\
&= (b_2 + \delta b_2)\ell_{22} + (b_3 + \delta b_3)\ell_{33} \\
\begin{pmatrix} \tilde{a}_2 & \tilde{a}_3 \end{pmatrix} &= \begin{pmatrix} b_2 + \delta b_2 & b_3 + \delta b_3 \end{pmatrix} L, \quad L = \tilde{R}^T
\end{aligned}$$

And what about BPR^T?

$BPT^T \equiv$ 

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$$\begin{aligned} \tilde{a}_3 &= (b_3 + \delta b_3)\ell_{33} \\ \tilde{a}_2 &= (b_2 + \delta_2 b_2)\ell_{22} + (b_3 + \delta_2 b_3)\ell_{32} \\ &= (b_2 + \delta_2 b_2)\ell_{22} + (b_3 + \delta b_3 - \delta b_3 + \delta_2 b_3) \\ &= (b_2 + \delta_2 b_2 + (\delta_2 b_3 - \delta b_3)\frac{\ell_{32}}{\ell_{22}})\ell_{22} + (b_3 + \delta b_3)\ell_{33} \\ &= (b_2 + \delta b_2)\ell_{22} + (b_3 + \delta b_3)\ell_{33} \\ \begin{pmatrix} \tilde{a}_2 & \tilde{a}_3 \end{pmatrix} &= \begin{pmatrix} b_2 + \delta b_2 & b_3 + \delta b_3 \end{pmatrix} L, \quad L = \tilde{R}^T \end{aligned}$$

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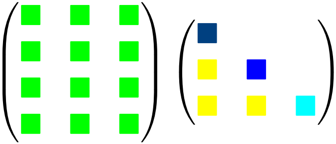
$BPT^T \equiv$ 

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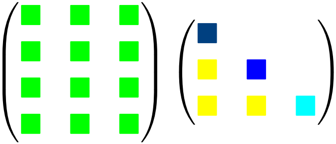
$BPT^T \equiv$ 

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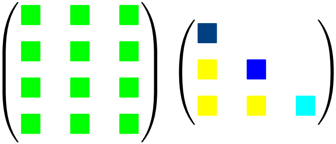
$$
\begin{aligned}
\tilde{a}_3 &= (b_3 + \delta b_3)\ell_{33} \\
\tilde{a}_2 &= (b_2 + \delta_2 b_2)\ell_{22} + (b_3 + \delta_2 b_3)\ell_{32} \\
&= (b_2 + \delta_2 b_2)\ell_{22} + (b_3 + \delta b_3 - \delta b_3 + \delta_2 b_3) \\
&= (b_2 + \delta_2 b_2 + (\delta_2 b_3 - \delta b_3)\frac{\ell_{32}}{\ell_{22}})\ell_{22} + (b_3 + \delta b_3)\ell_{33} \\
&= (b_2 + \delta b_2)\ell_{22} + (b_3 + \delta b_3)\ell_{33} \\
\begin{pmatrix} \tilde{a}_2 & \tilde{a}_3 \end{pmatrix} &= \begin{pmatrix} b_2 + \delta b_2 & b_3 + \delta b_3 \end{pmatrix} L, \quad L = \tilde{R}^T
\end{aligned}
$$

And what about BPR^T?

$BPT^T \equiv$ 

Consider $\begin{pmatrix} a_1 & a_2 & a_3 \end{pmatrix} = \begin{pmatrix} b_1 & b_2 & b_3 \end{pmatrix} \begin{pmatrix} \ell_{11} & 0 & 0 \\ \ell_{21} & \ell_{22} & 0 \\ \ell_{31} & \ell_{32} & \ell_{33} \end{pmatrix}$

$$\begin{aligned}
\tilde{a}_3 &= (b_3 + \delta b_3)\ell_{33} \\
\tilde{a}_2 &= (b_2 + \delta_2 b_2)\ell_{22} + (b_3 + \delta_2 b_3)\ell_{32} \\
&= (b_2 + \delta_2 b_2)\ell_{22} + (b_3 + \delta b_3 - \delta b_3 + \delta_2 b_3) \\
&= (b_2 + \delta_2 b_2 + (\delta_2 b_3 - \delta b_3)\frac{\ell_{32}}{\ell_{22}})\ell_{22} + (b_3 + \delta b_3)\ell_{33} \\
&= (b_2 + \delta b_2)\ell_{22} + (b_3 + \delta b_3)\ell_{33} \\
\begin{pmatrix} \tilde{a}_2 & \tilde{a}_3 \end{pmatrix} &= \begin{pmatrix} b_2 + \delta b_2 & b_3 + \delta b_3 \end{pmatrix} L, \quad L = \tilde{R}^T
\end{aligned}$$

Backward stability

- $C = Q \begin{pmatrix} R \\ 0 \end{pmatrix}$;
  - $C + \delta C = \tilde{Q} \begin{pmatrix} \tilde{R} \\ 0 \end{pmatrix}$;
  - $\|\delta C(:,i)\| \leq \epsilon \|C(:,i)\|$, for all columns i
- $A = BR^T$;
  - $\tilde{A} = (B + \delta B)\tilde{R}^T$,
  - $\|\delta B(:,i)\| \leq \epsilon \|B(:,i)\|$, for all columns i
- $(B + \delta B)(C + \delta C)^T = (I + \delta B B^\dagger) B C^T (I + \delta C C^\dagger)^T$
- $B = B_{scaled} D$, $scond(B) = cond(B_{scaled})$

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- $A = BR^T$;
  - $\tilde{A} = (B + \delta B)\tilde{R}^T$,
  - $\|\delta B(:, i)\| \leq \epsilon \|B(:, i)\|$, for all columns i
- $(B + \delta B)(C + \delta C)^T = (I + \delta BB^{\dagger})BC^T(I + \delta CC^{\dagger})^T$
- $B = B_{scaled}D$, $scond(B) = cond(B_{scaled})$

Backward stability

- $C = Q \begin{pmatrix} R \\ 0 \end{pmatrix}$;
  - $C + \delta C = \tilde{Q} \begin{pmatrix} \tilde{R} \\ 0 \end{pmatrix}$;
  - $\|\delta C(:,i)\| \leq \epsilon \|C(:,i)\|$, for all columns i
- $A = BR^T$;
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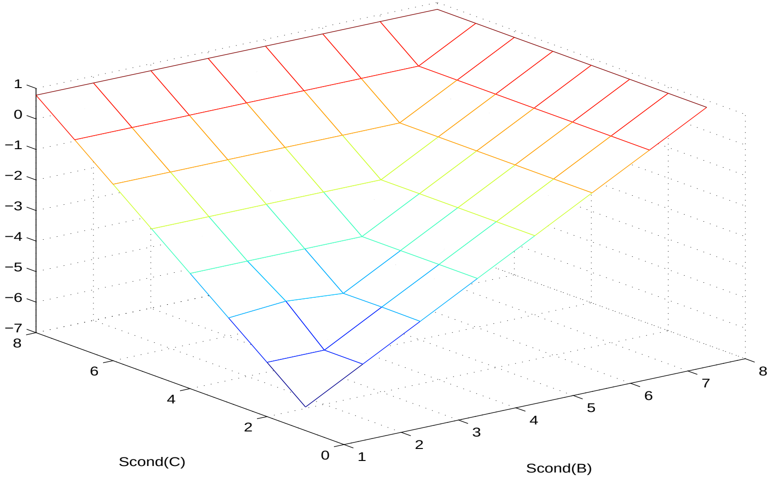
  - $\|\delta B(:,i)\| \leq \epsilon \|B(:,i)\|$, for all columns i
- $(B + \delta B)(C + \delta C)^T = (I + \delta B B^\dagger) B C^T (I + \delta C C^\dagger)^T$
- $B = B_{scaled} D$, $scond(B) = cond(B_{scaled})$

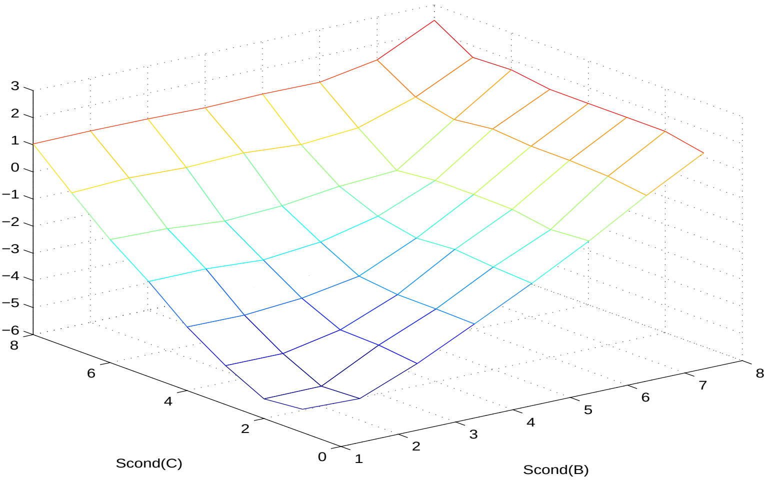
Theoretical accuracy



theory:

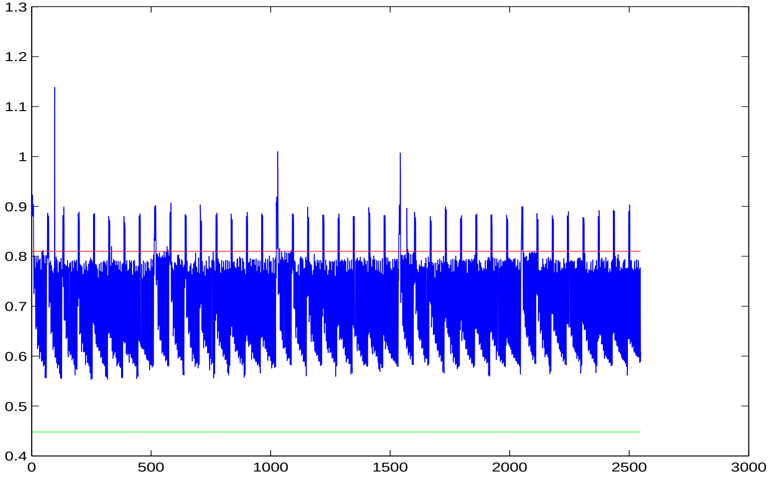
$$\max_i \frac{|\tilde{\sigma}_i - \sigma_i|}{\sigma_i} \leq f(m,p,n) \cdot \mathfrak{e} \cdot \max\{scond(B), scond(C)\}$$

Measured accuracy



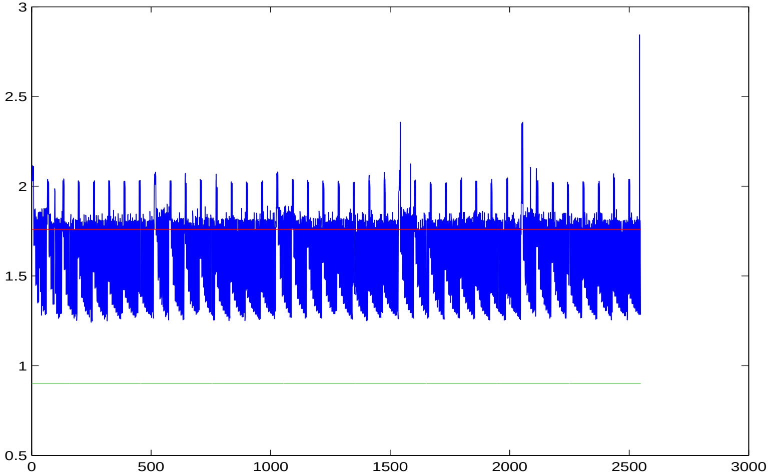
theory: measured $\max_i \frac{|\tilde{\sigma}_i - \sigma_i|}{\sigma_i}$; in $(0.3, 46)\times$ theory

Timings



$400 \times 350 \times 400$, *PSVD*, *SGESDD* ∘ *SGEMM*, *SGESVD* ∘ *SGEMM*

Timings



$500 \times 500 \times 500$, *PSVD*, *SGESDD* ∘ *SGEMM*, *SGESVD* ∘ *SGEMM*

Conclusion

- New implementation of Businger–Golub QRCP more reliable than xGEQP3 and equally efficient. Recommended as replacement for xGEQP3.
- Jacobi SVD code in final stage of testing.
- New Jacobi SVD code as basis for
  - SEVP $Hx = x\lambda$, SSVD
  - PSVD, $HMx = x\lambda$, $|\delta H_{ij}| \leq \epsilon\sqrt{H_{ii}H_{jj}}$
  - QSVD, $Hx = Mx\lambda$
  - (H, K)–SVD