

Solving Total Least Squares Problems Using Mixed Precision

SIAM CSE23

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Least-Squares Problems (LSP)

Goal : Solve $\min_x \|b - Ax\|_2$, where $A \in \mathbb{R}^{m \times n}$ ($m \geq n$) has rank n

Solve : QR factorization - $A = QR = [Q_1 \quad Q_2] \begin{bmatrix} U \\ 0 \end{bmatrix}$, where $Q \in \mathbb{R}^{m \times m}$ is orthogonal, and $U \in \mathbb{R}^{n \times n}$ is upper triangular.

$$Ax = b \rightarrow [Q_1 \quad Q_2] \begin{bmatrix} U \\ 0 \end{bmatrix} x = b \rightarrow x = U^{-1} Q_1^T b, \|b - Ax\|_2 = \|Q_2^T b\|_2$$

Normal Equations : $A^T Ax = A^T b \rightarrow \begin{bmatrix} I & A \\ A^T & 0 \end{bmatrix} \begin{bmatrix} r \\ x \end{bmatrix} = \begin{bmatrix} b \\ 0 \end{bmatrix}$

Mixed Precision LSP

Mixed precision IR is often used to solve least squares problems.

- Solve $Ax = b$
- Improve accuracy of the computed approximate solution \hat{x}
- Compute x_0 by GEPP

Algorithm: IR [Wilkinson, 1963]

```

 $Ax_0 = b$                                 in precision  $u_f$ ; store in precision  $u$ 
for  $i = 0 : i_{max} - 1$  do
     $r_i = b - Ax_i$                         in precision  $u_r$ ; store in precision  $u$ 
     $Ad_{i+1} = r_i$                         in precision  $u_s$ ; store in precision  $u$ 
     $x_{i+1} = x_i + d_{i+1}$                   in precision  $u$ 
    if converged then
        return  $x_{i+1}$ 
    end
end

```

Mixed Precision LSP

Mixed precision IR solves augmented system or normal equations.

Augmented system :

- [Björck, 1967] : Two precision IR
- [Demmel et al., 2009] : Two precision LSIR with BLAS
- [Carson et al., 2020] : Three precision GMRES-LSIR

Normal equations :

- [Yamazaki et al., 2015] : Mixed precision Cholesky
- [Higham and Pranesh, 2021] : Low precision Cholesky preconditioner in GMRES-LSIR and CG-LSIR

Total Least Squares Problems (TLSP)

Standard linear model : $Ax = b + r$, r - random error vector

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How realistic is this ?

Total Least Squares Problems (TLSP)

Standard linear model : $Ax = b + r$, r - random error vector

How realistic is this ?

Errors-in variables model : $(A + E)x = b + r$, E - random error matrix

Total Least Squares Problems (TLSP)

The first numerically stable algorithm ([Golub and Van Loan, 1980]).

$$\min_{E,r} \|[E; r]\|_F, (A + E)x = b + r$$

How to Solve TLSP ?

- **Direct methods** : Singular value decomposition

$[A; b] = U\Sigma V^T$, $\Sigma = \text{diag}(\sigma_1, \dots, \sigma_{n+1})$, with
 $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_{n+1} \geq 0$ and $V = [v_1, \dots, v_{n+1}]$.

Assume $\text{rank}(A)=n$. If $\sigma_{n+1} = 0$, then $[E; r] = 0$. If $\sigma_{n+1} > 0$, then
 $\min_{\text{rank}(A+E, b+r) < n+1} \|[E; r]\|_F = \sigma_{n+1}$ and

$$x_{TLS} = -\frac{1}{v_{n+1, n+1}} [v_{1, n+1}, \dots, v_{n, n+1}]^T.$$

How to Solve TLSP ?

- **Direct methods** : Singular value decomposition

$$[A; b] = U\Sigma V^T, \Sigma = \text{diag}(\sigma_1, \dots, \sigma_{n+1}), \text{ with } \sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_{n+1} \geq 0 \text{ and } V = [v_1, \dots, v_{n+1}].$$

Assume $\text{rank}(A)=n$. If $\sigma_{n+1} = 0$, then $[E; r] = 0$. If $\sigma_{n+1} > 0$, then $\min_{\text{rank}(A+E, b+r) < n+1} \|[E; r]\|_F = \sigma_{n+1}$ and

$$x_{TLS} = -\frac{1}{v_{n+1, n+1}} [v_{1, n+1}, \dots, v_{n, n+1}]^T.$$

- **Iterative methods** : Inverse iteration, (inverse) Chebyshev iteration [Van Huffel, 1991], **Rayleigh-quotient iteration (RQI)** [Björck, 1997], block Golub-Kahan bidiagonalization [Hnětynková et al., 2013]

Rayleigh-Quotient Iteration (RQI)

Algorithm: RQI

Given $x^{(0)}$ with $\|x^{(0)}\| = 1$

$$\rho^{(0)} = (x^{(0)})^T B x^{(0)}$$

for $k=1,2,\dots$ **do**

$$(B - \rho^{(k-1)} I)\omega = x^{(k-1)}$$

$$x^{(k)} = \omega / \|\omega\|$$

$$\rho^{(k)} = (x^{(k)})^T B x^{(k)}$$

end

- Inverse iteration with shift ρ - Rayleigh quotient to estimate eigenpair
- Given eigenvector x of B , estimate the corresponding eigenvalue.
- Rayleigh quotient - $\rho(x) = \frac{x^T B x}{x^T x}$
- Continually improve eigenvalue estimates to increase the rate of convergence of inverse iteration at each step.

RQI for TLSP

Eigenvalue problem : $\lambda = \sigma_{n+1}^2$ and $x = x_{TLS}$ satisfy

$$\begin{bmatrix} A^T A & A^T b \\ b^T A & b^T b \end{bmatrix} \begin{bmatrix} x \\ -1 \end{bmatrix} = \lambda \begin{bmatrix} x \\ -1 \end{bmatrix}$$

or

$$\begin{bmatrix} A^T \\ b^T \end{bmatrix} (-r) = \lambda \begin{bmatrix} x \\ -1 \end{bmatrix}, \text{ with } r = b - Ax.$$

Newton's method : $\begin{bmatrix} f(x, \lambda) \\ g(x, \lambda) \end{bmatrix} = \begin{bmatrix} -A^T r - \lambda x \\ -b^T r + \lambda \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$

Normal equations : $(A^T A - \sigma_{n+1}^2 I)x = A^T b$

RQI for TLSP

Rayleigh quotient :
$$\rho(x) = \frac{(x^T A^T - b^T)(Ax - b)}{x^T x + 1} = \frac{r^T r}{x^T x + 1}$$

The next approximation :
$$\begin{bmatrix} J^{(k)} & A^T b \\ b^T A & \eta_k \end{bmatrix} \begin{bmatrix} x^{(k+1)} \\ -1 \end{bmatrix} = \beta_k \begin{bmatrix} x^{(k)} \\ -1 \end{bmatrix},$$

with $J^{(k)} = A^T A - \rho_k I$, $\eta_k = b^T b - \rho_k$, β_k - scaling factor

RQI for TLSP

Algorithm: RQI for TLSP [Björck et al., 2000]

$$x = x_{LS}$$

$$r = b - Ax$$

$$\rho^2 = r^T r / (1 + x^T x)$$

$$\text{Solve } A^T A u = x$$

$$x = x + \rho^2 u$$

for $k=1,2,\dots$ **do**

$$r = b - Ax$$

$$\rho^2 = r^T r / (1 + x^T x)$$

$$f = -A^T r - \rho^2 x$$

$$g = -b^T r + \rho^2$$

$$\text{solve } (A^T A - \rho^2 I) \omega = -f$$

$$z = x + \omega$$

$$\beta = (z^T f - g) / (z^T x + 1)$$

$$\text{solve } (A^T A - \rho^2 I) u = x$$

$$x = z + \beta u$$

end

RQI for TLSP

Algorithm: RQI for TLSP [Björck et al., 2000]

```

 $x = x_{LS}$ 
 $r = b - Ax$ 
 $\rho^2 = r^T r / (1 + x^T x)$ 
Solve  $A^T A u = x$ 
 $x = x + \rho^2 u$ 
for  $k=1,2,\dots$  do
   $r = b - Ax$ 
   $\rho^2 = r^T r / (1 + x^T x)$ 
   $f = -A^T r - \rho^2 x$ 
   $g = -b^T r + \rho^2$ 
  solve  $(A^T A - \rho^2 I)\omega = -f$ 
   $z = x + \omega$ 
   $\beta = (z^T f - g) / (z^T x + 1)$ 
  solve  $(A^T A - \rho^2 I)u = x$ 
   $x = z + \beta u$ 
end

```



One step of inverse iteration

RQI for TLSP

Algorithm: RQI for TLSP [Björck et al., 2000]

```

 $x = x_{LS}$ 
 $r = b - Ax$ 
 $\rho^2 = r^T r / (1 + x^T x)$ 
Solve  $A^T A u = x$ 
 $x = x + \rho^2 u$ 

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← One step of inverse iteration

```

for  $k=1,2,\dots$  do
   $r = b - Ax$ 
   $\rho^2 = r^T r / (1 + x^T x)$ 
   $f = -A^T r - \rho^2 x$ 
   $g = -b^T r + \rho^2$ 
  solve  $(A^T A - \rho^2 I)\omega = -f$ 
   $z = x + \omega$ 
   $\beta = (z^T f - g) / (z^T x + 1)$ 
  solve  $(A^T A - \rho^2 I)u = x$ 
   $x = z + \beta u$ 

```

How to solve ?

end

RQI-PCGTLS

If $(A^T A - \rho^2 I)$ is SPD \rightarrow Use conjugate gradient! (with $k + 1$ iterations)

Preconditioner : Cholesky factor R of $A^T A$

RQI-PCGTLS

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Rayleigh Quotient Iteration with Preconditioned Conjugate Gradient
for TLS problems (RQI-PCGTLS) [Björck et al., 2000]

RQI-PCGTLS

Algorithm: PCGTLS for $(A^T A - \rho^2 I)\omega = f$ [Björck et al., 2000]

Initialize $\omega^{(0)} = 0$, $p^{(0)} = s^{(0)} = R^{-T} f$, $\eta_0 = \|s^{(0)}\|_2^2$

for $j=0, 1, \dots, l$, **while** $\delta_j \neq 0$ **do**

$$q^{(j)} = R^{-1} p^{(j)}$$

A is not used at all!

$$\delta_j = \|p^{(j)}\|_2^2 - \rho^2 \|q^{(j)}\|_2^2$$

$$\alpha_j = \eta_j / \delta_j$$

$$\omega^{(j+1)} = \omega^{(j)} + \alpha_j q^{(j)}$$

$$s^{(j+1)} = s^{(j)} - \alpha_j (p^{(j)} - \rho^2 q^{(j)})$$

$$\eta_{j+1} = \|s^{(j+1)}\|_2^2$$

$$\beta_j = \eta_{j+1} / \eta_j$$

$$p^{(j+1)} = s^{(j+1)} + \beta_j p^{(j)}$$

Assuming R is computed exactly,

$\tilde{C} = I - \rho^2 R^{-T} R^{-1}$ is the
preconditioned matrix.

end

Rayleigh-Quotient Iteration (RQI)

Algorithm: RQI-PCGTLS [Björck et al., 2000]

$$x = x_{LS}$$

$$r = b - Ax$$

$$\rho^2 = r^T r / (1 + x^T x)$$

Compute $A^T A$ and its Cholesky factor

$$\text{Solve } A^T A u = x$$

$$x = x + \rho^2 u$$

for $k=1,2,\dots$ **do**

$$r = b - Ax$$

$$\rho^2 = r^T r / (1 + x^T x)$$

$$f = -A^T r - \rho^2 x$$

$$g = -b^T r + \rho^2$$

$A^T A$ and Cholesky can be expensive !

$$\text{solve } (A^T A - \rho^2 I) \omega = -f$$

$$z = x + \omega$$

$$\beta = (z^T f - g) / (z^T x + 1)$$

$$\text{solve } (A^T A - \rho^2 I) u = x$$

$$x = z + \beta u$$

end

Rayleigh-Quotient Iteration (RQI)

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$$\text{solve } (A^T A - \rho^2 I) u = z$$

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end

$A^T A$ and Cholesky can be expensive !

Use lower precision !

- 1 Least-Squares Problems
- 2 Total Least-Squares Problems
- 3 RQI and RQI-PCGTLS
- 4 RQI-PCGTLS-MP**

Algorithm: RQI-PCGTLS [Björck et al., 2000]

$$x = x_{LS}$$

$$r = b - Ax$$

$$\rho^2 = r^T r / (1 + x^T x)$$

Compute $A^T A$ and its Cholesky factor

$$\text{Solve } A^T A u = x$$

$$x = x + \rho^2 u$$

for $k=1,2,\dots$ **do**

$$r = b - Ax$$

$$\rho^2 = r^T r / (1 + x^T x)$$

$$f = -A^T r - \rho^2 x$$

$$g = -b^T r + \rho^2$$

Solve $(A^T A - \rho^2 I)\omega = -f$ with PCGTLS

$$z = x + \omega$$

$$\beta = (z^T f - g) / (z^T x + 1)$$

Solve $(A^T A - \rho^2 I)u = x$ with PCGTLS

$$x = z + \beta u$$

end

Algorithm: RQI-PCGTLS-MP

$$x = x_{LS}$$

$$r = b - Ax$$

in precision u_r

$$\rho^2 = r^T r / (1 + x^T x)$$

Compute $A^T A$ and its Cholesky factorin precision u_c

$$\text{Solve } A^T A u = x$$

$$x = x + \rho^2 u$$

for $k=1,2,\dots$ **do**

$$r = b - Ax$$

$$\rho^2 = r^T r / (1 + x^T x)$$

in precision u

$$f = -A^T r - \rho^2 x$$

$$g = -b^T r + \rho^2$$

Solve $(A^T A - \rho^2 I)\omega = -f$ with PCGTLSin precision u_p

$$z = x + \omega$$

$$\beta = (z^T f - g) / (z^T x + 1)$$

Solve $(A^T A - \rho^2 I)u = x$ with PCGTLSin precision u_p

$$x = z + \beta u$$

end

Mixed Precision RQI-PCGTLS (RQI-PCGTLS-MP)

Use four precision in RQI-PCGTLS :

u_r - residual precision,

u - RQI working precision (store the data and solution),

u_p - PCGTLS working precision (store the data and solution),

u_c - $A^T A$ and Cholesky precision,

with $u_r \leq u \leq u_p \leq u_c$.

In this study we are using $(u_r, u, u_p, u_c) = (\text{quad}, \text{double}, \text{single}, \text{half})$.

Mixed Precision RQI-PCGTLS (RQI-PCGTLS-MP)

Termination criteria : Stop when the normalized residual norm increases ($\gamma_{k+1} > \gamma_k$) :

$$\gamma_k = \left(\frac{\|f_k\|_2^2 + g_k^2}{\|x^{(k)}\|_2^2 + 1} \right)^{1/2}$$

Necessary conditions for RQI-PCGTLS : Assume $\sigma'_1 \geq \sigma'_2 \geq \dots \geq \sigma'_n \geq 0$ are the singular values of A . Then,

[Björck, 1996] : $\sigma'_n > \sigma_{n+1} \Rightarrow x_{TLS}$ is unique.

[Björck et al., 2000] : $A^T A - \rho^2 I$ is SPD \Rightarrow PCGTLS is convergent.

Mixed Precision RQI-PCGTLS (RQI-PCGTLS-MP)

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[Björck et al., 2000] : $A^T A - \rho^2 I$ is SPD \Rightarrow PCGTLS is convergent.

Using [Demmel, 1989, Higham and Pranesh, 2021] :

$$\frac{\sigma_n'^2}{(2\sigma_n'^2 + n)(n+1)} > u_c, \quad \text{where } A^T A \in \mathbb{R}^{n \times n}.$$

Numerical Experiments - Van Huffel matrix, $n = 100$

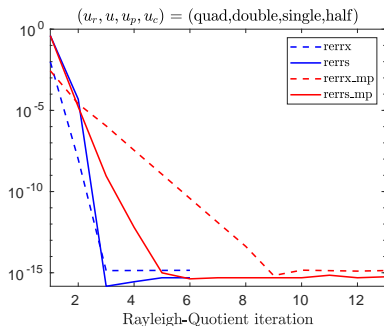
[Van Huffel and Vandewalle, 1991]

$$(A + E)x = b + e, \quad \epsilon = 10^{-6}$$

E - $\epsilon \times$ random matrix

e - $\epsilon \times$ random vector

$$\underbrace{\begin{bmatrix} n-1 & -1 & \cdots & -1 \\ -1 & n-1 & \cdots & -1 \\ \cdot & & & \\ \cdot & & & \\ \cdot & & & \\ -1 & -1 & \cdots & n-1 \\ -1 & -1 & \cdots & -1 \\ -1 & -1 & \cdots & -1 \end{bmatrix}}_{n \times n-2} \begin{bmatrix} x_1 \\ \cdot \\ \cdot \\ \cdot \\ x_{n-3} \\ x_{n-2} \end{bmatrix} \approx \begin{bmatrix} -1 \\ -1 \\ \cdot \\ \cdot \\ \cdot \\ -1 \\ n-1 \\ -1 \end{bmatrix}$$



Numerical Experiments - Toeplitz matrix, $n = 100$

$$(\bar{T} + E)x = \bar{g} + e, \quad \epsilon = 10^{-6}$$

$$\gamma_{\bar{T}} = 0.001 \|\bar{T}\|, \quad \gamma_{\bar{g}} = 0.001 \|\bar{g}\|$$

\bar{g} - vector of ones,

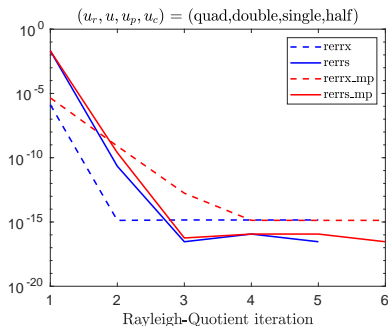
E - $\epsilon \times \gamma_{\bar{T}} \times$ random Toeplitz matrix,

e - $\epsilon \times \gamma_{\bar{g}} \times$ random vector

$\bar{T}^{n \times (n-2\omega)}$ - lower Toeplitz matrix

$$t_{i,1} = \begin{cases} \frac{1}{\sqrt{2\pi\alpha^2}} e^{\left[-\frac{(\omega-i+1)^2}{2\alpha^2}\right]} & i = 1, 2, \dots, 2\omega + 1, \\ 0 & \text{otherwise,} \end{cases}$$

$$t_{1,j} = \begin{cases} t_{1,1} & \text{if } j = 1, \\ 0 & \text{otherwise,} \end{cases} \quad \text{with } \alpha = 1.25, \omega = 2$$



Conclusion

- Forming $A^T A$ and Cholesky factorization can dominate the computational cost.
- Use as low precision as possible to decrease the computational cost.
- The precision for factorization depends on σ'_n .
- RQI-PCGTLS-MP converges to the same level as RQI-PCGTLS
- Using low precision increases the number of RQI

Conclusion

- Forming $A^T A$ and Cholesky factorization can dominate the computational cost.
- Use as low precision as possible to decrease the computational cost.
- The precision for factorization depends on σ'_n .
- RQI-PCGTLS-MP converges to the same level as RQI-PCGTLS
- Using low precision increases the number of RQI **but performance can compensate the additional iterations !**

Next Step...


- Performance analysis with larger sized matrices
- Complete theoretical analysis of RQI-PCGTLS-MP by adapting, e.g.,
 - Results on inexact Newton in [Higham and Mary, 2022, Tisseur, 2001, Kelley, 2022],
 - Results on inexact RQI in [Freitag and Spence, 2007, Simoncini and Eldén, 2002].


Complete analysis includes :


- Proof of attainable accuracy,
- Theoretical explanation of different convergence delay.


Thank you for your attention !


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SIAM Journal on Scientific Computing, 37(3) :C307–C330.

More examples - δ matrix, $\delta = 10^{-2}$

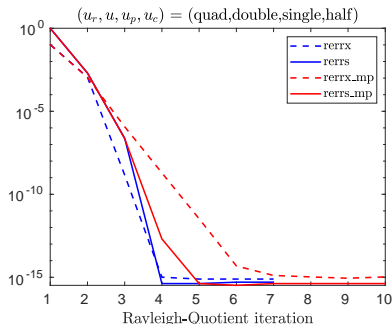
$$(A + E)x = b + e,$$

$$E = 10^{-8}\bar{E} \cdot A, \quad e = 10^{-8}\bar{e} \cdot b$$

\bar{E} - random matrix,

\bar{e} - random vector

$$\begin{bmatrix} \delta & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & \delta & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ x_9 \end{bmatrix} = \begin{bmatrix} 1 \\ 1 \\ \cdot \\ \cdot \\ \cdot \\ \cdot \\ 1 \end{bmatrix}$$



More examples - Random matrix, $m = 100, n = 60$

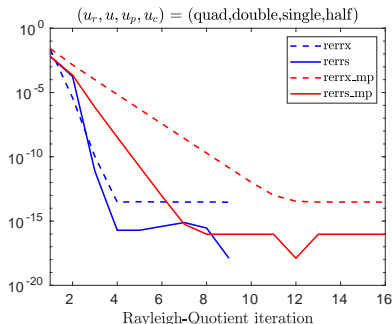
$(A + E)x = b + e$, where

$A \in \mathbb{R}^{m \times n}$ - random matrix,

$b \in \mathbb{R}^m$ - vectors of ones,

$E = 10^{-6}\bar{E}$, $e = 10^{-6}\bar{e}$

\bar{E} - random matrix, \bar{e} - random vector



More examples - [Björck et al., 1998], $m = 30, n = 15$

Used to test the convergence properties of
RQI-PCGTLS

$(A + E)x = b + e$, where

$E = 0.05\bar{E}$, $e = 0.05\bar{e}$

\bar{E} - random matrix, \bar{e} - random vector

$b = Ax$ with $x = (1, 1/2, \dots, 1/n)$,

$A = Y \begin{bmatrix} D \\ 0 \end{bmatrix} Z^T \in \mathbb{R}^{m \times n}$, where

Y, Z - random orthogonal matrices

$D = \text{diag}(1, 2^{-1}, \dots, 2^{-n+1})$

