Solving the Indefinite Least Squares Problem by Hyperbolic QR Factorization

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Definition

$$\min_x (b - Ax)^T J (b - Ax),$$

where $A \in \mathbb{R}^{m \times n}$, $m \geq n$, and

$$J = \begin{bmatrix} I_p & 0 \\ 0 & -I_q \end{bmatrix}, \qquad p + q = m.$$

Normal equations:

$$A^T J A x = A^T J b.$$

Unique solution iff

$A^T J A$ positive definite.

This condition implies

- $p \geq n$
- A has full rank.

Application: Total Least Squares

$$\min \left\{ \| [A\ b] - [\widetilde{A}\ \widetilde{b}] \|_F^2 : \widetilde{A}, \widetilde{b} \in R(\widetilde{A}) \right\}$$

Assume

$$\sigma_{\min}(A) = \sigma_n > \overline{\sigma}_{n+1} = \sigma_{\min}([A\ b]).$$

Then there is a unique TLS solution:

$$x_{\text{TLS}} = (A^T A - \overline{\sigma}_{n+1}^2 I_n)^{-1} A^T b.$$

x_{TLS} minimizes the indefinite cost function

$$\|b - Ax\|_2^2 - \overline{\sigma}_{n+1}^2 \|x\|_2^2 = r(x)^T \begin{bmatrix} I_m & 0 \\ 0 & -I_n \end{bmatrix} r(x),$$

where

$$r(x) = \begin{bmatrix} b \\ 0 \end{bmatrix} - \begin{bmatrix} A \\ \overline{\sigma}_{n+1} I_n \end{bmatrix} x.$$

QR-Cholesky Method

Chandrasekaran, Gu & Sayed (1998): factorize

$$A = QR = \begin{matrix} & n \\ p & \\ q & \end{matrix}\begin{bmatrix} Q_1 \\ Q_2 \end{bmatrix} R, \qquad R \in \mathbb{R}^{n \times n}, \quad Q^T Q = I.$$

Normal equations $A^T J A x = A^T J b$ become

$$R^T Q^T J Q R x = R^T Q^T J b, \qquad \text{or} \qquad (Q_1^T Q_1 - Q_2^T Q_2) R x = Q^T J b.$$

1. Form $C = Q_1^T Q_1 - Q_2^T Q_2$.
2. Cholesky factorize $C = U^T U$.
3. Solve $U^T U R x = Q^T J b$.

Cost: $n^2(5m - n)$ flops.

Hyperbolic QR Method

Hyperbolic QR factorization:

$$Q^T A = \begin{bmatrix} R \\ 0 \end{bmatrix}, \quad R \in \mathbb{R}^{n\times n}, \qquad Q^T J Q = J.$$

Then

$$\begin{aligned}(b - Ax)^T J (b - Ax) &= (b - Ax)^T Q J Q^T (b - Ax) \\ &= \begin{bmatrix} c_1 - Rx \\ c_2 \end{bmatrix}^T J \begin{bmatrix} c_1 - Rx \\ c_2 \end{bmatrix} \\ &= \|c_1 - Rx\|_2^2 + c_2^T J(n+1\colon m, n+1\colon m) c_2.\end{aligned}$$

We compute:

$$A = \begin{matrix} & n \\ p & \begin{bmatrix} A_1 \\ A_2 \end{bmatrix} \\ q & \end{matrix} \xrightarrow{\text{Householder}} \begin{matrix} & n \\ p & \begin{bmatrix} R_1 \\ A_2 \end{bmatrix} \\ q & \end{matrix} \xrightarrow{\text{hyperbolic}} \begin{matrix} & n \\ n & \begin{bmatrix} R \\ 0 \end{bmatrix} \\ m-n & \end{matrix}.$$

Hyperbolic Rotations

$$H = \begin{bmatrix} c & -s \\ -s & c \end{bmatrix}, \qquad c^2 - s^2 = 1.$$

Assuming $|x_1| > |x_2|$, can compute

$$\begin{bmatrix} r \\ 0 \end{bmatrix} = \begin{bmatrix} c & -s \\ -s & c \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$
$$= \begin{bmatrix} 1 & 0 \\ -s/c & 1/c \end{bmatrix} \begin{bmatrix} c & -s \\ 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}.$$

- Using factored (“mixed”) form advantageous for stability (Bojanczyk et al., 1987).

Example

$m = 6$, $n = p = q = 3$.

$$
\begin{bmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{bmatrix}
\xrightarrow{P_1}
\begin{bmatrix} \times & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \\ \times & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \end{bmatrix}
\xrightarrow{H_{14}}
\left[\begin{array}{c|cc} \times & \times & \times \\ \hline 0 & \times & \times \\ 0 & 0 & \times \\ 0 & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \end{array}\right]
$$

$$
\xrightarrow{P_2}
\left[\begin{array}{c|cc} \times & \times & \times \\ \hline 0 & \times & \times \\ 0 & 0 & \times \\ 0 & \times & \times \\ 0 & 0 & \times \\ 0 & 0 & \times \end{array}\right]
\xrightarrow{H_{24}}
\left[\begin{array}{c|cc} \times & \times & \times \\ \hline 0 & \times & \times \\ 0 & 0 & \times \\ 0 & 0 & \times \\ 0 & 0 & \times \\ 0 & 0 & \times \end{array}\right]
\longrightarrow \cdots \longrightarrow
\left[\begin{array}{ccc} \times & \times & \times \\ 0 & \times & \times \\ 0 & 0 & \times \\ \hline 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{array}\right]
$$

- Existence of hyperbolic rotations proved using definiteness of $A^T J A$.

Operation Counts

	Normal eqns	Hyperbolic QR	QR-Cholesky
	$n^2(m + n/3)$	$2n^2(m - n/3)$	$n^2(5m - n)$
$m \approx n$	$4n^3/3$	$4n^3/3$	$4n^3$
$m \gg n$	mn^2	$2mn^2$	$5mn^2$

QR-Cholesky proved backward stable by Chandrasekaran, Gu & Sayed (1998).

Error Analysis: First Attempt

Consider

$$y = H_k H_{k-1} \dots H_1 x,$$

where H_i is an $n \times n$ hyperbolic transformation.
In floating point,

$$y = (H_k + \Delta H_k)(H_{k-1} + \Delta H_{k-1}) \dots (H_1 + \Delta H_1)x,$$
$$|\Delta H_i| \le \gamma_n |H_i|.$$

Does not lead to useful result, because $\|H_i\|$ unbounded.

Hyperbolic $\leftrightarrow$ Orthogonal

Let Q be J-orthogonal and

$$A = \begin{matrix} \\ p \\ q \end{matrix} \overset{n}{\begin{bmatrix} A_1 \\ A_2 \end{bmatrix}} = \begin{matrix} \\ p \\ q \end{matrix} \begin{matrix} p & q \\ \left[\begin{matrix} Q_{11} \\ Q_{21} \end{matrix}\right. & \left.\begin{matrix} Q_{12} \\ Q_{22} \end{matrix}\right] \end{matrix} \overset{n}{\begin{bmatrix} B_1 \\ B_2 \end{bmatrix}} \begin{matrix} \\ p \\ q \end{matrix} = QB.$$

Then

$$\begin{bmatrix} B_1 \\ A_2 \end{bmatrix} = \mathrm{exc}(Q) \begin{bmatrix} A_1 \\ B_2 \end{bmatrix},$$

where

$$\mathrm{exc}(Q) = \begin{bmatrix} Q_{11}^{-1} & -Q_{11}^{-1}Q_{12} \\ Q_{21}Q_{11}^{-1} & Q_{22} - Q_{21}Q_{11}^{-1}Q_{12} \end{bmatrix}$$

is orthogonal. In fact,

$$\mathrm{exc}(\mathrm{exc}(P)) = P.$$

Combining Non-Overlapping Hyperbolic Transformations

$$\begin{bmatrix} R \\ S \\ X \end{bmatrix} \begin{matrix} t \\ p-t \\ q \end{matrix} \quad \xrightarrow{H_{23}} \begin{bmatrix} R \\ S_1 \\ X_1 \end{bmatrix} \xrightarrow{H_{13}} \begin{bmatrix} R_1 \\ S_1 \\ X_2 \end{bmatrix}.$$

Using exc relation,

$$G_1 \begin{bmatrix} S_1 \\ X \end{bmatrix} = \begin{bmatrix} S \\ X_1 \end{bmatrix}, \qquad G_2 \begin{bmatrix} R_1 \\ X_1 \end{bmatrix} = \begin{bmatrix} R \\ X_2 \end{bmatrix},$$

for orthogonal G_i. Incorporating errors gives

$$G_1 \begin{bmatrix} S_1 + E_1 \\ X + E_2 \end{bmatrix} = \begin{bmatrix} S \\ X_1 \end{bmatrix}, \qquad G_2 \begin{bmatrix} R_1 + F_1 \\ X_1 + F_2 \end{bmatrix} = \begin{bmatrix} R \\ X_2 \end{bmatrix}.$$

Can be manipulated into

$$\begin{bmatrix} R_1 \\ S_1 \\ X \end{bmatrix} + \Delta = G \begin{bmatrix} R \\ S \\ X_2 \end{bmatrix},$$

with “commensurate” bounds on Δ.

Analysis of One Rotation

Computed

$$\begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \begin{bmatrix} c & -s \\ -s & c \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

satisfi es

$$\begin{bmatrix} x_1 \\ \widehat{y}_2 \end{bmatrix} = G \begin{bmatrix} \widehat{y}_1 + e_1 \\ x_2 + e_2 \end{bmatrix},$$

where

$$G = \begin{bmatrix} 1/c & s/c \\ -s/c & 1/c \end{bmatrix},$$

$$\max(|e_1|, |e_2|) \leq \gamma_6 \max(|\widehat{y}_1|, |x_2|),$$

with $\gamma_n = nu/(1 - nu)$.

- Mixed backward–forward stability result.

Stability of Hyperbolic QR Factorization

$$\begin{array}{c} \\ p \\ q \end{array} \overset{n}{\begin{bmatrix} A_1 \\ A_2 \end{bmatrix}} = Q \begin{array}{c} \\ p \\ q \end{array} \overset{n}{\begin{bmatrix} R_1 \\ 0 \end{bmatrix}}.$$

Computed $\widehat{R}_1$ satisfies

$$\begin{bmatrix} \widehat{R}_1 + \Delta_3 \\ A_2 + \Delta_2 \end{bmatrix} = G \begin{bmatrix} A_1 + \Delta_1 \\ 0 \end{bmatrix}, \qquad G^T G = I,$$

$$\|\Delta_1\|_F \le \widetilde{\gamma}_{pn} \|A_1\|_F,$$

$$\|\Delta_i\|_F \le \widetilde{\gamma}_{qn} \max(\|\widehat{R}_1\|_F, \|A_2\|_F) \quad i = 2\colon 3.$$

Equivalently,

$$\begin{bmatrix} A_1 + \Delta_1 \\ A_2 + \Delta_2 \end{bmatrix} = Q \begin{bmatrix} \widehat{R}_1 + \Delta_3 \\ 0 \end{bmatrix}, \qquad Q^T J Q = J.$$

Can prove backward stability if $\kappa_2(A_1) u = O(1)$.

Perturbation Theory

Let $x + \Delta x$ solve

$$\min_x (b + \Delta b - (A + \Delta A)x)^T J (b + \Delta b - (A + \Delta A)x),$$

where

$$\|\Delta A\|_F \leq \epsilon \|\mathbf{A}\|_F, \quad \|\Delta b\|_2 \leq \epsilon \|\mathbf{b}\|_2.$$

Can show

$$\frac{\|\Delta x\|_2}{\|x\|_2} \leq \epsilon \Bigg[\|M^{-1} A^T\|_2 \|\mathbf{A}\|_F \left(\frac{\|\mathbf{b}\|_2}{\|\mathbf{A}\|_F \|x\|_2} + 1 \right) + \|M^{-1}\|_2 \|A\|_F^2 \frac{\|\mathbf{A}\|_F}{\|A\|_F} \frac{\|r\|_2}{\|A\|_F \|x\|_2} \Bigg] + O(\epsilon^2).$$

Conjecture: This bound is nearly attainable.

Solving the ILS problem

- ★ Now consider transformations on RHS (again in “exc form”).
- ★ Bound forward error by sum of: error in final triangular solve, error in solution of certain perturbed ILS problem.
- ★ Error bound contains
  - growth in transformed RHS
  - inverse of R
- ★ Both can be bounded in terms of problem condition number (assuming conjecture true)
  $\Rightarrow$ hyperbolic QR method is forward stable.

Numerical Experiment

$$A = \begin{matrix} p \\ q \end{matrix} \begin{bmatrix} Q_1 DU \\ \frac{1}{2} Q_2 DU \end{bmatrix},$$

where U, Q_1,Q_2 random orthogonal, $D = \mathrm{diag}(\kappa^{-1}, \ldots, 1)$.
$x \in N(0,1)$, $b := Ax$.

In every case $\|r\|_2/(\|A\|_2\|x\|_2) \approx u$,
$\|Q\|_2 = 1.73$, $\|Q^T A - [R^T\ 0]^T\|_2/\|A\|_2 \approx u$, $\|Q^T J Q - J\|_2 \leq 10u$.

κ	Hyperbolic QR	QR-Cholesky	Normal equations	$\mathrm{cond} \times u$
10^2	4.9e-15	4.0e-15	2.0e-13	2.1e-14
10^6	3.0e-11	1.7e-11	2.6e-5	1.9e-10
10^{10}	9.7e-8	1.5e-7	2.4e0	1.3e-6
10^{12}	4.8e-4	9.8e-3	6.4e0	1.4e-2

Conclusions

- Gave perturbation analysis for ILS problem and identifi ed condition number.
  - Question over attainability of a perturbation bound.
- New method for ILS problem based on hyperbolic QR.
  - Lower operation count.
  - Method is forward stable, despite large-normed transformations.
- New insight into error analysis of product of hyperbolic transformations: non-overlapping, use of exc operator.
- Currently extending the work to ILS problem with linear equality constraints.

`http://www.ma.man.ac.uk/~nareports/narep397.ps.gz`