Stability and Sensitivity of LSP Solutions

Backward stability of matrix-vector & matrix-matrix multiplication

Let V be any $n \times n$ invertible matrix and x be any nonzero column vector of length n. Then the following hold in floating point arithmetic.

(a) $\mathrm{fl}(Vx) = Vx + b$ where $|b| \leq \gamma |V||x|$, with γ satisfying $|\gamma| \leq nu + O(u^2)$.

(b) $\mathrm{fl}(Vx) = V(x + \delta x)$ where $|\delta x| \leq \gamma |V^{-1}||V||x|$ and $\|\delta x\|_1 \leq \gamma \kappa_1(V) \|x\|_1$ for a scalar γ satisfying $|\gamma| \leq nu + O(u^2)$.

(c) Given any $n \times n$ matrix A, there exists an $n \times n$ matrix δA, such that $\mathrm{fl}(VA) = V(A + \delta A)$ with $|\delta A_j| \leq \gamma |V^{-1}||V||A_j|$, for a scalar γ (which does not depend on j) such that $|\gamma| \leq nu + O(u^2)$ for all $j = 1, \ldots, n$, where A_j and δA_j are the j^{th} columns of A and δA respectively.

Further, $\frac{\|\delta A\|_2}{\|A\|_2} \leq n \frac{\|\delta A\|_1}{\|A\|_1} \leq n^2 \beta \kappa_2(V)$ for a scalar β such that $|\beta| \leq nu + O(u^2)$.

Stability of orthogonal matrix multiplication

Multiplication of an $n \times n$ orthogonal matrix Q to any $n \times m$ matrix A is a backward stable computation, i.e., for any

$$fl(Q * A) = Q * (A + \Delta) \text{ where } \|\Delta\|_2 / \|A\|_2 \approx cu$$

for some small scalar c.

Hence, for $n \geq m$, the upper triangular matrix $fl(R)$ of the QR decomposition of A computed via application of rotators or reflectors to A satisfies

$$A + \Delta = Q * fl(R)$$

where $\|\Delta\|_2 / \|A\|_2 \approx \alpha u$ for some small scalar α and Q is the same as the Q of a QR decomposition of A.

Stability of QR method

The LSP solution of an overdetermined system $Ax = b$ via QR decomposition with $\operatorname{rank} A = r$ is obtained from the following steps:

1. Find $R = \begin{bmatrix} R_1 & R_2 \\ 0 & 0 \end{bmatrix}$ of a rank revealing QR decomposition of A and suppose $Q_1, \ldots, Q_r$ are the reflectors and $P_1, \ldots P_r$ are the permutations required in the process. Here $r \leq m$.
2. Compute $c = Q_r \cdots Q_1 b$ and extract vectors c_1, c_2 from its first entries.
3. Solve $R_1 y = c_1$.
4. Set $x_0 = P_1 \cdots P_r \begin{bmatrix} y \\ 0 \end{bmatrix}_{m \times 1}$.

Since all the steps are backward stable, finding the LSP solution of $Ax = b$ via QR decomposition is the LSP solution of a system $(A + \Delta)x = b + \delta b$ where $\|\Delta\|_2 / \|A\|_2$ and $\|\delta b\|_2 / \|b\|_2$ are small multiples of u.

Stability of SVD method

The LSP solution of an overdetermined system $Ax = b$ via SVD method in the full rank case is obtained from the following steps:

(i) Computed the condensed SVD $A = U_r \Sigma_r V_r^T$.

(ii) Compute $c = V_r \Sigma_r^{-1} U_r^T b$.

Each of the steps are backward stable. So finding the LSP solution of $Ax = b$ computed via the SVD of A is the LSP solution of a system $(A + \Delta)x = b + \delta b$ where $\|\Delta\|_2 / \|A\|_2$ and $\|\delta b\|_2 / \|b\|_2$ are small multiples of u.

Stability of Normal Equations Method

If A is full rank, the LSP solution say x_c of $Ax = b$ computed via the Normal Equations Method satisfies

$$(A^T A + \Delta)x_c = A^T b + c$$

where $\|\Delta\|_2 / \|A\|_2^2 \leq \gamma_{n,m} u$ and $\|c\|_2 / \|b\|_2 \leq \alpha_{n,m} u \|A\|_2$ for constants $\gamma_{n,m}$ and $\alpha_{n,m}$ depending on n and m.

However this is not equivalent to x_c being the solution of $(A + \Delta)^T (A + \Delta) x_c = (A + \Delta)^T (b + \delta b)$ where $\|\Delta\|_2 / \|A\|_2$ and $\|\delta b\|_2 / \|b\|_2$ are small multiples of u unless A is very well conditioned.

Therefore there is no guarantee that x_c is an LSP solution of $(A + \Delta)x = (b + \delta b)$ for some small enough $\|\Delta\|_2 / \|A\|_2$ and $\|\delta b\|_2 / \|b\|_2$. Hence the Normal Equations Method of solving the LSP *need not be backward stable.*

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Sensitivity of LSP solution

Let $A \in \mathbb{R}^{n\times m}$, $n \geq m$ such that $\operatorname{rank} A = m$. Let $b \in \mathbb{R}^n$. Then the unique Least Square Solution of $x_0 \in \mathbb{R}^m$ $Ax = b$ satisfies

$$\|Ax_0 - b\|_2 = \min_{x\in\mathbb{R}^m} \|Ax - b\|_2.$$

The sensitivity of x_0 to changes in A and b will measure the relative change in x_0 with respect to the relative perturbations to A and b.

The finding of x_0 is a two stage process, viz.,

(I) Find $y_0 \in R(A)$, such that $\|b - y_0\|_2 = \min_{y\in R(A)} \|b - y\|_2$.

(II) Find $x_0 \in \mathbb{R}^m$ such that $Ax_0 = y_0$.

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Perturbing only b

Let x be the unique LSP solution of $Ax = b$ with $\operatorname{rank} A = m$. Let $y := Ax$ and $r := b - Ax$ If θ be the angle between b and y, then

(a) $\|r\|_2 = \|b\|_2 \sin\theta$.

(b) $\|y\|_2 = \|b\|_2 \cos\theta$.

Now let $x + \delta x$ be the unique LSP solution of $Ax = b + \delta b$. Let $\hat{y} := A(x + \delta x)$ and $\hat{r} := (b + \delta b) - A(x + \delta x)$. If $\delta y := \hat{y} - y$ and $\delta r := \hat{r} - r$, then

(i) $\delta b = \delta r + \delta y$.

(ii) $(\delta r)^T (\delta y) = 0$.

(iii) $\|\delta y\|_2 \leq \|\delta b\|_2$.

(iv) If $\cos\theta \neq 0$, $\frac{\|\delta y\|_2}{\|y\|_2} \leq \frac{1}{\cos\theta} \frac{\|\delta b\|_2}{\|b\|_2}$.

(v) $\frac{\|\delta x\|_2}{\|x\|_2} \leq \kappa_2(A) \frac{\|\delta y\|_2}{\|y\|_2}$.

(vi) $\frac{\|\delta x\|_2}{\|x\|_2} \leq \frac{\kappa_2(A)}{\cos\theta} \frac{\|\delta b\|_2}{\|b\|_2}$. Ex: Prove (a), (b) and (i) - (vi)

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Perturbing both A and b

Theorem Let $A, A + \Delta A \in \mathbb{R}^{n\times m}$ with $n \geq m$ and $\operatorname{rank} A = \operatorname{rank} A + \Delta A = m$. Let x and $x + \delta x$ be the LSP solutions of $Ax = b$ and $(A + \Delta A)w = b + \delta b$ where $b, \delta b \in \mathbb{R}^n$. Also let $r = Ax - b$ and $r + \delta r = (A + \Delta A)(x + \delta x) - b + \delta b$. If $\|\Delta A\|_2 \leq \epsilon \|A\|_2$ and $\|\delta b\|_2 \leq \epsilon \|b\|_2$ where $\epsilon < 1/\kappa_2(A)$, then

$$\begin{aligned}
\frac{\|\delta x\|_2}{\|x\|_2} &\leq \frac{\kappa_2(A)\epsilon}{1 - \kappa_2(A)\epsilon}\left(2 + (\kappa_2(A) + 1)\frac{\|r\|_2}{\|A\|_2\|x\|_2}\right), \\
\frac{\|\delta r\|_2}{\|b\|_2} &\leq (1 + 2\kappa_2(A))\epsilon.
\end{aligned}$$

The upper bounds in the above sensitivity analysis will apply to the forward errors associated with the solutions and residuals computed via QR and SVD methods as they are backward stable.

However the forward error of the LSP solution via Normal Equations Method satisfies

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QR vs Normal Equations (NE)

- QR is always backward stable.
- Forward error of NE method can be more than that via QR if A is ill conditioned and residual is small.
- The solution via QR can be iteratively refined. But the same when applied to the solution via NE is slow to converge as the rate of convergence depends on $\kappa_2(A)^2$.