Componentwise inclusion for solutions in least squares problems and underdetermined systems

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Problems considered

- Least squares (LS) problems

$$\min_{x \in \mathbb{R}^n} \|b - Ax\|_2, \qquad A \in \mathbb{R}^{m \times n}, \quad b \in \mathbb{R}^m, \quad m \geq n$$

LS solution $= A^+ b$

- Underdetermined systems (US)

$$Ax = b, \qquad A \in \mathbb{R}^{n \times m}, \quad b \in \mathbb{R}^n, \quad m \geq n$$

Minimal 2-norm solution $= A^+ b$

Purpose

Numerically computing componentwise enclosure for $A^{+}b$

$\Rightarrow$ Numerically computing vector r satisfying $|\tilde{x} - A^{+}b| \leq r$ for approximate solutions $\tilde{x}$

Preferable

- Smaller error bounds
- Fast algorithm

Previous Work

LS	normwise	componentwise
fast	Rump (2012)	?
not fast		Rohn (2009), Rump (1999)

US	normwise	componentwise
fast	Miyajima (2010), Rump (2012)	?
not fast		Rohn (2009), Rump (1999)

Our contribution

- Algorithm for computing componentwise error bounds of $\tilde{x}$
- do not assume but prove A to have full rank
- Similar computational cost to that of Rump (2012)
- Theory showing that the obtained error bounds by the proposed algorithms are equal or smaller than those by Rump (2012)

Rump's bound in LS (1/2)

$A \approx QR$: an economy size approximate QR factorization.

$S \approx R^{-1}$.

AS can be expected to be not too far from orthogonality.

Theorem 1 [Rump (2012)] Let

- $A \in \mathbb{R}^{m \times n}$, $\tilde{x} \in \mathbb{R}^n$, $\tilde{w}, b \in \mathbb{R}^m$, $S \in \mathbb{R}^{n \times n}$, $p \in \{1, 2, \infty\}$
- $X := AS$, $\rho_{\tilde{x}} := A\tilde{x} - \tilde{w} - b$, $\rho_{\tilde{w}} := A^T\tilde{w}$

Rump's bound in LS (2/2)

If $\|I_n - X^T X\|_p \le \alpha_p < 1$, A has full rank, $\|\tilde{x} - A^+ b\|_p \le \delta_p$, $\|\tilde{x} - A^+ b\|_p \le \varepsilon_p$, $\|\tilde{x} - A^+ b\|_2 \le \zeta$, where

$$\delta_p := \frac{\|S\|_p}{1-\alpha_p}\left(\|X^T \rho_{\tilde{x}}\|_p + \|S^T \rho_{\tilde{w}}\|_p\right),$$

$$\varepsilon_p := \|SX^T \rho_{\tilde{x}}\|_p + \|SS^T \rho_{\tilde{w}}\|_p + \frac{\alpha_p \|S\|_p}{1-\alpha_p}\left(\|X^T \rho_{\tilde{x}}\|_p + \|S^T \rho_{\tilde{w}}\|_p\right),$$

$$\zeta := \|SX^T \rho_{\tilde{x}}\|_2 + \|SS^T \rho_{\tilde{w}}\|_2 + \frac{\alpha_2 \|S\|_2 \|\rho_{\tilde{w}}\|_2}{\sqrt{1-\alpha_2}} + \frac{\alpha_2 \|S\|_2}{1-\alpha_2}\|S^T \rho_{\tilde{w}}\|_2.$$

Proposed bound in LS

Theorem 2 Let $e^{(n)} := (1, \ldots, 1)^T$, $E := I_n - X^T X$. Assume $|E| \le \Gamma$, $\|\Gamma\|_p \le \alpha_p < 1$. Then A has full rank, S is nonsingular, $|\tilde{x} - A^+ b| \le q$, $|\tilde{x} - A^+ b| \le r^{(p)}$, $|\tilde{x} - A^+ b| \le s$, where

$$q := |SS^T(A^T\rho_{\tilde{x}} + \rho_{\tilde{w}})| + \frac{\|S^T(A^T\rho_{\tilde{x}} + \rho_{\tilde{w}})\|_\infty}{1 - \alpha_\infty}|S|\Gamma e^{(n)},$$

$$r^{(p)} := |SS^T(A^T\rho_{\tilde{x}} + \rho_{\tilde{w}})| + \frac{\alpha_p\|S\|_p\|S^T(A^T\rho_{\tilde{x}} + \rho_{\tilde{w}})\|_p}{1 - \alpha_p}e^{(n)},$$

$$s := |SS^T(A^T\rho_{\tilde{x}} + \rho_{\tilde{w}})| + \alpha_2\|S\|_2\left(\frac{\|\rho_{\tilde{x}}\|_2}{\sqrt{1 - \alpha_2}} + \frac{\|S^T\rho_{\tilde{w}}\|_2}{1 - \alpha_2}\right)e^{(n)}.$$

Relations between the bounds

Theorem 3 $q \le r^{(\infty)}, \quad \max_{1 \le i \le n} r_i^{(p)} \le \varepsilon_p \le \delta_p, \quad \max_{1 \le i \le n} s_i \le \zeta.$

Numerical examples in LS

Intel Xeon 2.66GHz Dual CPU, 4.00GB RAM, MATLAB 7.5 with Intel MKL, and IEEE 754 double precision

`P = qr(A,0); R = triu(P(1:n,:));` S `= R\speye(n);`
$\tilde{x}$ `= A\b;` $\tilde{w}$ `= A*(`S`*(`S`'*(A'*b)))-b;`

- M1: The algorithm computing q in the proposed bound
- M2: M1 with iterative refinement
- R1: The algorithm computing ε_∞ in Rump's bound
- R2: R1 with iterative refinement
- I: INTLAB function `verifylss`
- V: Versoft function `verlsq`

Example 1 [Obtained error bounds] (1/3)

```
A = gallery('randsvd',[200,100],cnd); b = randn(200,1);
```

cnd	M1			M2		
	max	mean	min	max	mean	min
1e+4	1.68e–3	9.99e–4	3.38e–4	4.25e–19	2.52e–19	8.56e–20
1e+6	8.09e+2	4.42e+2	1.56e+2	2.04e–13	1.12e–13	3.94e–14
1e+8	4.42e+8	2.17e+8	7.39e+7	1.13e–7	5.56e–8	1.89e–8
1e+10	3.15e+14	1.51e+14	4.88e+13	7.86e–2	3.78e–2	1.22e–2
1e+12	2.40e+20	1.07e+20	3.27e+19	5.92e+4	2.64e+4	8.10e+3
1e+14	fail1	fail1	fail1	fail1	fail1	fail1

fail1: $\alpha_\infty < 1$ could not be verified

Example 1 [Obtained error bounds] (2/3)

`cnd`	R1	R2
1e+4	1.68e–3	4.27e–13
1e+6	8.09e+2	3.50e–11
1e+8	4.42e+8	1.15e–7
1e+10	3.17e+14	7.93e–2
1e+12	2.50e+20	6.15e+4
1e+14	fail1	fail1

fail1: $\alpha_\infty < 1$ could not be verified

Example 1 [Obtained error bounds] (3/3)

cnd	I			V		
	max	mean	min	max	mean	min
1e+4	6.88e–11	2.72e–11	8.80e–12	2.63e–6	1.47e–6	7.08e–7
1e+6	3.04e–7	1.09e–7	2.05e–8	1.95e–2	9.86e–3	3.80e–3
1e+8	1.92e–3	6.10e–4	8.34e–5	1.68e+2	7.61e+1	2.53e+1
1e+10	1.62e+1	6.29e+0	1.66e+0	1.42e+6	6.14e+5	1.78e+5
1e+12	1.13e+5	3.73e+4	4.09e+3	1.32e+10	5.29e+9	1.33e+9
1e+14	3.04e+9	1.09e+9	2.39e+8	1.77e+14	6.57e+13	1.50e+13

Example 2 [computing times (sec)]

```
A = randn(m,n); b = randn(m,1);
```

m	n	M1	M2	R1	R2	I	V
600	100	0.02	0.05	0.02	0.05	0.59	3.38
700	100	0.03	0.08	0.03	0.08	0.86	4.95
800	100	0.03	0.09	0.03	0.09	1.19	6.94
400	100	0.01	0.03	0.01	0.03	0.25	1.34
400	200	0.04	0.10	0.04	0.10	0.39	2.11
400	300	0.09	0.18	0.09	0.20	0.60	3.29

Example 3 [computing times (sec)]

`A = randn(m,n); b = randn(m,1);` MO: memory over

m	n	M1	M2	R1	R2	I	V
5000	100	0.22	0.75	0.21	0.75	MO	MO
6000	100	0.27	0.93	0.26	0.93	MO	MO
7000	100	0.35	1.12	0.34	1.16	MO	MO
8000	100	0.45	1.38	0.43	1.38	MO	MO
4000	100	0.17	0.60	0.17	0.59	MO	MO
4000	200	0.48	1.40	0.47	1.39	MO	MO
4000	300	0.99	2.42	0.98	2.42	MO	MO
4000	400	1.68	3.62	1.67	3.59	MO	MO

Rump's bound in US (1/2)

$A^T \approx QR$: an economy size approximate QR factorization.

$S \approx R^{-T}$.

SA can be expected to be not too far from orthogonality.

Theorem 4 [Rump (2012)] Let

- $A \in \mathbb{R}^{n \times m}$, $\tilde{x} \in \mathbb{R}^m$, $\tilde{w}, b \in \mathbb{R}^n$, $S \in \mathbb{R}^{n \times n}$, $\hat{p} \in \{1, \infty\}$
- $Y := SA$, $\rho_{\tilde{w}} := \tilde{x} - A^T \tilde{w}$, $\rho_{\tilde{x}} := A\tilde{x} - b$

Rump's bound in US (2/2)

If $\|I_n - YY^T\|_p \le \alpha_p < 1$, A has full rank, $\|\tilde{x} - A^+b\|_{\hat{p}} \le \nu_{\hat{p}}$, $\|\tilde{x} - A^+b\|_2 \le \omega$, where

$$\nu_{\hat{p}} := \sqrt{m}\|\rho_{\tilde{w}}\|_{\hat{p}} + \|Y^T S\rho_{\tilde{x}}\|_{\hat{p}} + \frac{\alpha_{\hat{p}}\|Y^T\|_{\hat{p}}\|S\rho_{\tilde{x}}\|_{\hat{p}}}{1-\alpha_{\hat{p}}},$$

$$\omega := \|\rho_{\tilde{w}}\|_2 + \|Y^T S\rho_{\tilde{x}}\|_2 + \frac{\alpha_2\|S\rho_{\tilde{x}}\|_2}{\sqrt{1-\alpha_2}}.$$

Proposed bound in US

Theorem 5 Let $F := I_n - YY^T$. Assume $|F| \le \Phi$, $\|\Phi\|_p \le \alpha_p < 1$. Then A has full rank, S is nonsingular, $|\tilde{x} - A^+b| \le t$, $|\tilde{x} - A^+b| \le u^{(\hat{p})}$, $|\tilde{x} - A^+b| \le v$, where

$$t := \|\rho_{\tilde{w}}\|_2 e^{(m)} + |Y^T S \rho_{\tilde{x}}| + \frac{\|S\rho_{\tilde{x}}\|_\infty}{1-\alpha_\infty} |Y^T| \Phi e^{(n)},$$

$$u^{(\hat{p})} := \|\rho_{\tilde{w}}\|_2 e^{(m)} + |Y^T S \rho_{\tilde{x}}| + \frac{\alpha_{\hat{p}} \|Y^T\|_{\hat{p}} \|S\rho_{\tilde{x}}\|_{\hat{p}}}{1-\alpha_{\hat{p}}} e^{(m)},$$

$$v := \|\rho_{\tilde{w}}\|_2 e^{(m)} + |Y^T S \rho_{\tilde{x}}| + \frac{\alpha_2 \|S\rho_{\tilde{x}}\|_2}{\sqrt{1-\alpha_2}} e^{(m)}.$$

Relations between the bounds

Theorem 6 $t \le u^{(\infty)}$, $\max_{1\le i\le m} u_i^{(\hat{p})} \le \nu_{\hat{p}}$, $\max_{1\le i\le m} v_i \le \omega$.

Numerical examples in US

```
P = qr(A',0); R = triu(P(1:n,:)); S = R'\speye(n);
w̃ = S'*(S*b); x̃ = A'*w̃;
```

M1: The algorithm computing t in the proposed bound
M2: M1 with iterative refinement
M3: Miyajima (2010) without iterative refinement
M4: Miyajima (2010) with iterative refinement
R1: The algorithm computing ν_∞ in Rump's bound
R2: R1 with iterative refinement
I: INTLAB function `verifylss`
V: Versoft function `verlsq`

Example 1 [Obtained error bounds] (1/3)

```
A = gallery('randsvd',[100,200],cnd); b = randn(100,1);
```

cnd	M1			M2		
	max	mean	min	max	mean	min
1e+4	1.49e–3	8.90e–4	4.76e–4	1.30e–12	1.14e–12	1.10e–12
1e+6	7.14e+2	3.86e+2	1.77e+2	1.09e–10	9.68e–11	9.32e–11
1e+8	4.16e+8	2.05e+8	8.15e+7	1.70e–7	8.99e–8	4.17e–8
1e+10	2.73e+14	1.28e+14	4.60e+13	1.00e–1	4.69e–2	1.69e–2
1e+12	2.06e+20	8.97e+19	2.99e+19	7.51e+4	3.28e+4	1.09e+4
1e+14	fail1	fail1	fail1	fail1	fail1	fail1

fail1: $\alpha_\infty < 1$ could not be verified

Example 1 [Obtained error bounds] (2/3)

cnd	M3	M4	R1	R2
1e+4	4.90e–7	1.88e–12	1.49e–3	4.75e–12
1e+6	3.13e–3	1.59e–10	7.14e+2	3.81e–10
1e+8	2.20e+1	1.58e–8	4.16e+8	1.95e–7
1e+10	1.70e+5	1.27e–6	2.73e+14	1.00e–1
1e+12	7.39e+9	4.41e–4	2.06e+20	7.51e+4
1e+14	fail2	fail2	fail1	fail1

fail1: $\alpha_\infty < 1$ could not be verified

fail2: nonsingularity of R could not be verified

Example 1 [Obtained error bounds] (3/3)

cnd	I			V		
	max	mean	min	max	mean	min
1e+4	3.46e–11	7.11e–12	2.66e–12	1.11e–6	7.38e–7	5.37e–7
1e+6	2.33e–7	2.90e–8	5.71e–9	7.88e–3	4.92e–3	3.33e–3
1e+8	1.63e–3	3.05e–4	8.83e–5	6.50e+1	3.77e+1	2.44e+1
1e+10	1.29e+1	2.05e+0	5.08e–1	5.54e+5	3.10e+5	1.96e+5
1e+12	1.07e+5	1.23e+4	2.54e+3	5.02e+9	2.66e+9	1.60e+9
1e+14	1.54e+9	2.85e+8	1.21e+8	6.32e+13	3.31e+13	1.94e+13

Example 2 [computing times (sec)]

```
A = randn(n,m); b = randn(m,1);
```

m	n	M1	M2	M3	M4	R1	R2
5000	100	0.18	0.72	0.19	3.21	0.15	1.27
6000	100	0.23	0.89	0.25	3.86	0.19	1.56
7000	100	0.28	1.06	0.32	4.53	0.25	1.85
8000	100	0.34	1.28	0.41	5.21	0.30	2.22
4000	100	0.14	0.57	0.16	2.58	0.12	0.99
4000	200	0.35	1.28	0.40	3.10	0.32	2.24
4000	300	0.65	2.11	0.75	3.77	0.59	3.57
4000	400	1.00	3.27	1.19	4.48	0.92	4.93