Bounds for the Matrix Condition Number

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Outline

- Condition number and preconditioning
- Extended Lanczos bidiagonalization: a lower bound for $\kappa(A)$
- A probabilistic upper bound for $\kappa(A)$
- Results and conclusions

Uses of $\kappa(A)$

Consider $A\mathbf{x} = \mathbf{b}, \quad A \in \mathbb{R}^{n\times n}, \quad A$ nonsingular.

Problem:

- A, $\mathbf{b}$ perturbed
- Compute $\mathbf{x} = A^{-1}\mathbf{b}$
- Accuracy solution $\mathbf{x}$?

Sensitivity of linear system:

$$\frac{\|\Delta\mathbf{x}\|}{\|\mathbf{x}\|} \leq \kappa(A)\left(\frac{\|\Delta A\|}{\|A\|} + \frac{\|\Delta\mathbf{b}\|}{\|\mathbf{b}\|}\right)$$

Uses of $\kappa(A)$

Consider $A\mathbf{x} = \mathbf{b}, \quad A \in \mathbb{R}^{n\times n}, \quad A$ symmetric positive definite.

Problem:

- Iteratively solve with CG (Conjugate Gradients).
- $\mathbf{x}_k$ approximate solution after k steps.
- Convergence rate?

After k steps

$$\|\mathbf{x} - \mathbf{x}_k\|_A \leq 2\left(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1}\right)^k \|\mathbf{x} - \mathbf{x}_0\|_A.$$

($\|x\|_A = (Ax, x)^{1/2}$)

How to compute the condition number?

Matrix 2-norm:

$$\|A\|_2 \;=\; \max_{x\neq 0} \frac{\|A\mathbf{x}\|_2}{\|\mathbf{x}\|_2} \;=\; \sigma_1(A) \;=\; \sqrt{\lambda_1(A^TA)} \;=\; \lambda_1\left(\begin{bmatrix} 0 & A^T \\ A & 0 \end{bmatrix}\right)$$

Matrix condition number:

$$\kappa(A) \;=\; \|A\|_2\,\|A^{-1}\|_2 \;=\; \frac{\sigma_1(A)}{\sigma_n(A)} \;=\; \sqrt{\frac{\lambda_1(A^TA)}{\lambda_n(A^TA)}}$$

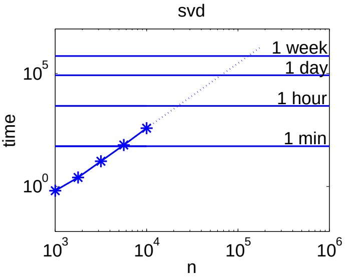
How to compute the condition number?

- Singular value decomposition (svd):

$A = X\Sigma Y^T,$

$$\text{where } \Sigma = \begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_n \end{bmatrix}.$$

- Computation: $\approx 21n^3$ flops
- Example: `A = rand(n);`



Approximate the condition number

- Approximate $\sigma_1(A)$ and $\sigma_n(A)$

Bounds for largest singular value

Lower bound θ:

- Krylov subspace methods (Lanczos bidiagonalization)

Upper bounds:

- Bauer-Fike theorem (1960): *There is a singular value in* $[\theta, \theta + C]$.
  - not guaranteed σ_1
- Probabilistic bound [Hochstenbach 2013]

Problem:

- Find upper and lower bound for smallest singular value

Focus on preconditioning

Goal:

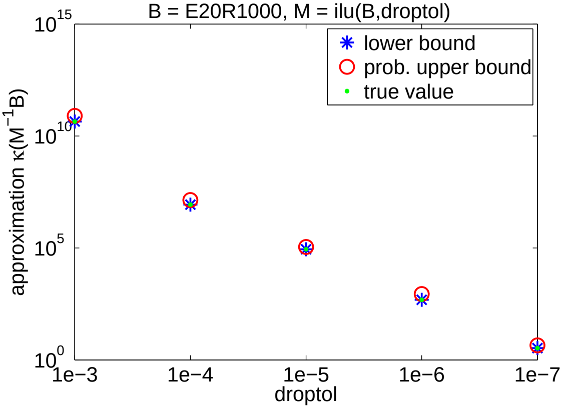
- Given: matrix B, preconditioner M
- Approximate: $\kappa(M^{-1}B)$

Proposed approach:

- Assumptions: LU-decomposition of B and M are available (and transposes)
- Output: lower bound and probabilistic upper bound for $\kappa(M^{-1}B)$

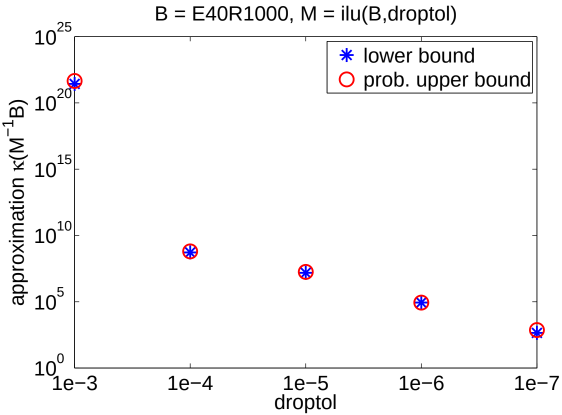
Example

- $\dim(B) = 4241$
- average time bounds:
  1.68 s
- total time true value:
  52 s
- $\kappa(B) = 3.3 \cdot 10^7$



Example

- $\dim(B) = 17281$
- average time bounds:
  24.28 s
- $\kappa(B) \approx 2.3 \cdot 10^8$



Bidiagonalization

Goal:

- A nonsymmetric, $\quad \sigma_i(A)^2 = \lambda_i(A^TA)$
- Find $\kappa(A) = \|A\| \, \|A^{-1}\| = \sqrt{\dfrac{\lambda_1(A^TA)}{\lambda_n(A^TA)}}$

Lanczos Bidiagonalization, procedure:

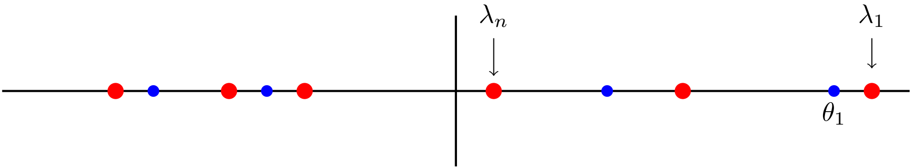
$$\mathbf{v}_0 \xrightarrow{A} \mathbf{u}_0 \xrightarrow{A^T} \mathbf{v}_1 \xrightarrow{A} \mathbf{u}_1 \xrightarrow{A^T} \ldots$$

Lanczos Bidiagonalization

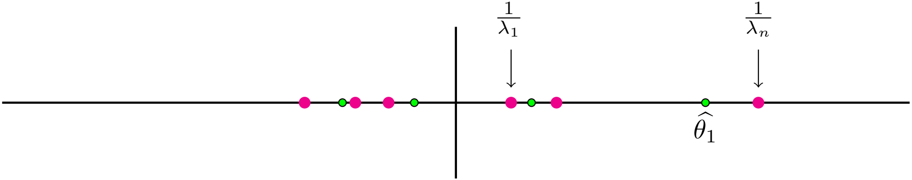
- $$\begin{aligned} AV_k &= U_k B_k \\ A^T U_k &= V_k B_k^T + \beta \mathbf{v}_{k+1} \mathbf{e}_k^T \end{aligned}$$
- $\mathbf{v}_k = p_k(A^T A)\mathbf{v}_0$
- $B_k = U_k^T A V_k$ bidiagonal
- Basis for Krylov subspace $\mathcal{K}_k(A^T A, \mathbf{v}_0)$.

Available theory:

- Lower bound for $\|A\|_2$
- Probabilistic upper bound for $\|A\|_2$ [Hochstenbach, 2013]
- Other examples: bounds for $\|M^{-1}B - I\|_2$



- eigenvalues of A
- approximations to eigenvalues of A



- eigenvalues of A^{-1}
- approximations to eigenvalues of A^{-1}

Extended Lanczos Bidiagonalization

Procedure:

$$\mathbf{v}_0 \xrightarrow{A} \mathbf{u}_0 \xrightarrow{A^T} \mathbf{v}_1 \xrightarrow{A^{-T}} \mathbf{u}_1 \xrightarrow{A^{-1}} \dots$$

Equations:

$$\begin{aligned} A^TAV &= VH^TH \\ (A^TA)^{-1}V &= VKK^T \\ AA^TU &= UHH^T \\ (AA^T)^{-1}U &= UK^TK \end{aligned}$$

$$\mathbf{v}_k = p_k(A^TA)\mathbf{v}_0$$
$$\mathbf{u}_k = q_k(AA^T)\mathbf{u}_0$$

Characteristics:

- H and K are tridiagonal, $H \cdot K = I$
- p_k and q_k are Laurent polynomials
- $\mathcal{K}_{m,m}(A^TA, \mathbf{v}_0) = \text{span}\{\dots, (A^TA)^{-1}\mathbf{v}_0, \mathbf{v}_0, A^TA\mathbf{v}_0, \dots\}$.

Proposition: The matrix H is tridiagonal and of the form

$$\begin{bmatrix} \alpha_0 & \beta_0 & & & & & \\ & \alpha_1 & & & & & \\ & \beta_{-1} & \alpha_{-1} & \beta_1 & & & \\ & & & \alpha_2 & & & \\ & & & \beta_{-2} & \alpha_{-2} & \beta_2 & \\ & & & & & \alpha_3 & \\ & & & & & & \ddots \end{bmatrix}, \qquad (1)$$

where its entries satisfy

$$\begin{aligned} h_{2j,2j} &= \alpha_j &&= \|A^{-T}\mathbf{v}_j\|^{-1} = \|A^T\mathbf{u}_{-j}\|, \\ h_{2j+1,2j} &= \beta_{-j} &&= \mathbf{u}_j^T A\mathbf{v}_j, \\ h_{2j+1,2j+1} &= \alpha_{-j} &&= \mathbf{u}_j^T A\mathbf{v}_{-j}, \\ h_{2j+1,2j+2} &= \beta_j &&= \|A^T\mathbf{u}_j - (\mathbf{u}_j^T A\mathbf{v}_j)\mathbf{v}_j - (\mathbf{u}_j^T A\mathbf{v}_{-j})\mathbf{v}_{-j}\|. \end{aligned}$$

Lower bound for $\kappa(A)$

Extended **Lanczos Bidiagonalization:**

- Largest singular value θ_1 of H approximates $\sigma_1(A)$
- Smallest singular value θ_k of H approximates $\sigma_n(A)$
- Lower bound for condition number:

$$\frac{\theta_1}{\theta_k} \leq \kappa(A)$$

Probabilistic upper bound

Available upper bounds:

- Bauer-Fike theorem (1960): *" There is a singular value in* $[\theta, \theta + C]$*, ... ".*
  - not guaranteed σ_1
- Probabilistic upper bound for $\|A\|_2$ [Hochstenbach 2013]
  - For preconditioning: bound for $\|M^{-1}B - I\|_2$.

Probabilistic upper bound

Let $\mathbf{v}_0 = \sum_{i=1}^{n} \gamma_i \mathbf{y}_i,$ $\qquad$ ($\mathbf{y}_i$ right singular vectors of A)

then

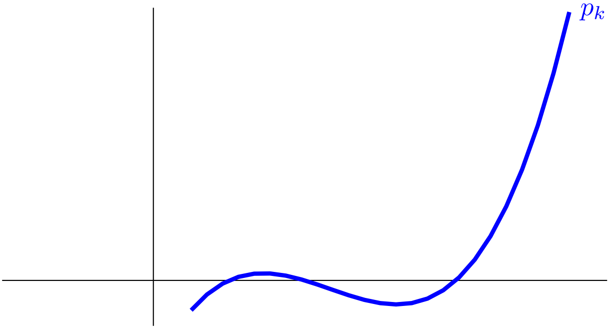
$$1 = \|\mathbf{v}_k\|^2 = \|p_k(A^TA)\mathbf{v}_0\|^2 = \sum_{i=1}^{n} \gamma_i^2 p_k(\sigma_i^2)^2.$$

Thus

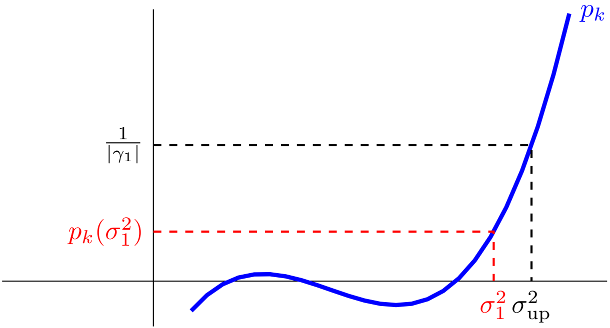
$$1 \geq \gamma_1^2\, p_k(\sigma_1^2)^2,$$

and

$$\frac{1}{|\gamma_1|} \geq |p_k(\sigma_1^2)|.$$



Recall: $\frac{1}{|\gamma_1|} \geq |p_k(\sigma_1^2)|$



Recall: $\frac{1}{|\gamma_1|} \geq |p_k(\sigma_1^2)|$

Question: $\mathbb{P}(\frac{1}{\delta} < \frac{1}{|\gamma_1|}) = \mathbb{P}(|\gamma_1| < \delta) = \epsilon$ (ϵ is user-chosen)

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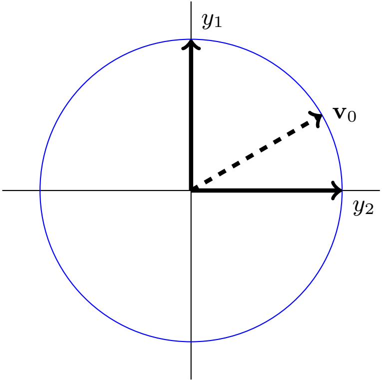
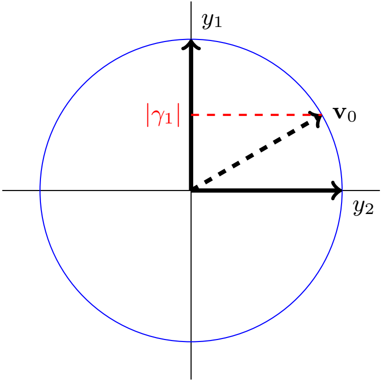
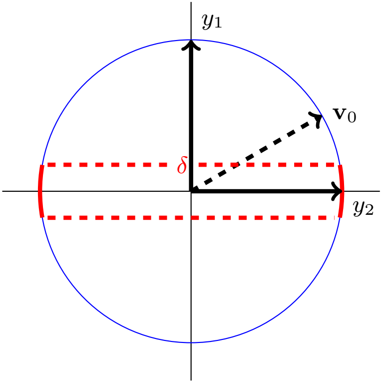


$\mathbb{P}(\frac{1}{\delta} < \frac{1}{|\gamma_1|}) = \mathbb{P}(|\gamma_1| < \delta) = \epsilon$ (ϵ is user-chosen)



$\mathbb{P}(\frac{1}{\delta} < \frac{1}{|\gamma_1|}) = \mathbb{P}(|\gamma_1| < \delta) = \epsilon$ (ϵ is user-chosen)



Theorem:

- starting vector $\mathbf{v}_0$ chosen randomly (uniform distribution over S^{n-1})
- $\varepsilon \in (0,1)$ user chosen
- δ be given by $\varepsilon = \mathcal{P}(\gamma_1 \leq \delta) = \dfrac{B_{\mathrm{inc}}(\frac{n-1}{2}, \frac{1}{2}, \delta^2)}{B_{\mathrm{inc}}(\frac{n-1}{2}, \frac{1}{2}, 1)}$,

where $B_{\mathrm{inc}}(x,y,z) = \int_0^z t^{x-1}(1-t)^{y-1} dt$ (incomplete Beta function)

Then $\sigma_{\mathrm{up}}^{\mathrm{prob}}$, the square root of the largest zero of the polynomial

$$f_1^{\delta}(t) = |p_k(t)| - \tfrac{1}{\delta},$$

is upper bound for σ_1 with probability at least $1-\varepsilon$.

User chosen values

- ε, probabilistic bound holds with probability at least $1 - 2\varepsilon$
- ζ, method adaptively performs k steps such that

$$\frac{\kappa_{\text{up}}}{\kappa_{\text{low}}} \leq \zeta$$

Bounds:

- probabilistic upper bound: $\kappa(A) \leq \frac{\sigma_1^{\text{prob}}}{\sigma_n^{\text{prob}}} = \kappa_{\text{up}}$
- deterministic lower bound: $\kappa_{\text{low}} = \frac{\theta_1}{\theta_k} \leq \kappa(A)$

Matrix B	droptol	Dim.	κ	κ_{low}	κ_{up}	k	CPU	LU
E20R1000	10^{-3}	4241	$4.44 \cdot 10^{10}$	$4.44 \cdot 10^{10}$	$7.96 \cdot 10^{10}$	4	1.47	69
	10^{-4}		$8.63 \cdot 10^{6}$	$8.63 \cdot 10^{6}$	$1.38 \cdot 10^{7}$	4	1.54	73
	10^{-5}		$8.72 \cdot 10^{4}$	$8.72 \cdot 10^{4}$	$1.11 \cdot 10^{5}$	4	1.73	72
	10^{-6}		$4.85 \cdot 10^{2}$	$4.84 \cdot 10^{2}$	$8.76 \cdot 10^{2}$	3	1.76	78
	10^{-7}		$3.35 \cdot 10^{0}$	$3.35 \cdot 10^{0}$	$4.48 \cdot 10^{0}$	3	1.82	79
E40R1000	10^{-3}	17281	$\star$	$2.73 \cdot 10^{21}$	$4.45 \cdot 10^{21}$	4	20.78	83
	10^{-4}		$\star$	$5.24 \cdot 10^{8}$	$6.38 \cdot 10^{8}$	4	23.28	84
	10^{-5}		$\star$	$1.53 \cdot 10^{7}$	$1.80 \cdot 10^{7}$	4	24.12	84
	10^{-6}		$\star$	$8.64 \cdot 10^{4}$	$8.73 \cdot 10^{4}$	4	26.12	84
	10^{-7}		$\star$	$4.46 \cdot 10^{2}$	$7.23 \cdot 10^{2}$	3	26.56	88

- Preconditioner: $M =$ `ilu(B,droptol)`
- For $\zeta = 2$ (i.e. $\kappa_{\text{up}}/\kappa_{\text{low}} \leq 2$)
- $\varepsilon = 0.01$ (i.e. upper bound holds with probability at least 98%)
- $\kappa(\texttt{e20r1000}) = 3.34 \cdot 10^{7}$
- Bounds for $\kappa(\texttt{e40r1000})$: $\kappa_{\text{low}} = 2.29 \cdot 10^{8}$ and $\kappa_{\text{up}} = 2.97 \cdot 10^{8}$

Matrix A	Dim.	κ	κ_{low}	κ_{up}	k	CPU	LU	CPU[1]
utm5940	5940	$4.35 \cdot 10^8$	$3.98 \cdot 10^8$	$7.21 \cdot 10^8$	4	0.13	61	0.12
grcar10000	10000	$3.63 \cdot 10^0$	$3.59 \cdot 10^0$	$5.80 \cdot 10^0$	6	0.07	31	0.05
af23560	23560	$1.99 \cdot 10^4$	$1.93 \cdot 10^4$	$2.82 \cdot 10^4$	6	0.98	74	0.88
rajat16	96294	$\star$	$5.63 \cdot 10^{12}$	$5.69 \cdot 10^{12}$	5	9.34	97	9.19
torso1	116158	$\star$	$1.41 \cdot 10^{10}$	$1.42 \cdot 10^{10}$	3	26.8	93	28.5
dc1	116835	$\star$	$2.39 \cdot 10^8$	$4.59 \cdot 10^8$	5	6.05	93	5.57
xenon2	157464	$\star$	$4.29 \cdot 10^4$	$8.14 \cdot 10^4$	7	20.1	82	19.6
scircuit	170998	$\star$	$2.40 \cdot 10^9$	$4.69 \cdot 10^9$	7	2.05	54	1.39
transient	178866	$\star$	$1.02 \cdot 10^{11}$	$2.00 \cdot 10^{11}$	8	7.70	86	7.12
stomach	213360	$\star$	$4.62 \cdot 10^1$	$9.02 \cdot 10^1$	6	13.8	80	13.7

- For $\zeta = 2$ (i.e. $\kappa_{\text{up}}/\kappa_{\text{low}} \leq 2$)
- $\varepsilon = 0.01$ (i.e. upper bound holds with probability at least 98%)
- CPU[1] indicates time of `condest`

Matrix A	Dim.	κ	κ_{low}	κ_{up}	k	CPU	LU
`utm5940`	5940	$4.35 \cdot 10^8$	$4.35 \cdot 10^8$	$4.71 \cdot 10^8$	10	0.19	42
`grcar10000`	10000	$3.63 \cdot 10^0$	$3.62 \cdot 10^0$	$3.97 \cdot 10^0$	13	0.13	21
`af23560`	23560	$1.99 \cdot 10^4$	$1.99 \cdot 10^4$	$2.12 \cdot 10^4$	9	1.14	66
`rajat16`	96294	$\star$	$5.63 \cdot 10^{12}$	$5.69 \cdot 10^{12}$	5	9.34	97
`torso1`	116158	$\star$	$1.41 \cdot 10^{10}$	$1.42 \cdot 10^{10}$	3	26.8	93
`dc1`	116835	$\star$	$2.39 \cdot 10^8$	$2.45 \cdot 10^8$	8	6.52	91
`xenon2`	157464	$\star$	$4.32 \cdot 10^4$	$4.67 \cdot 10^4$	14	23.6	70
`scircuit`	170998	$\star$	$2.45 \cdot 10^9$	$2.67 \cdot 10^9$	16	3.28	33
`transient`	178866	$\star$	$1.03 \cdot 10^{11}$	$1.11 \cdot 10^{11}$	21	9.47	70
`stomach`	213360	$\star$	$4.82 \cdot 10^1$	$5.24 \cdot 10^1$	14	17.5	63

- For $\zeta = 1.1$ (i.e. $\kappa_{\text{up}}/\kappa_{\text{low}} \leq 1.1$)
- $\varepsilon = 0.01$ (i.e. upper bound holds with probability at least 98%)

Conclusions

Bounds for the condition number:

- lower bound: $\kappa_{\text{low}} = \frac{\theta_1}{\theta_k} \leq \kappa(A)$
- probabilistic upper bound: $\kappa(A) \leq \frac{\sigma_1^{\text{prob}}}{\sigma_n^{\text{prob}}} = \kappa_{\text{up}}$

User chosen values:

- ε, probabilistic bound holds with probability at least $1 - 2\varepsilon$
- ζ, method adaptively performs k steps such that

$$\frac{\kappa_{\text{up}}}{\kappa_{\text{low}}} \leq \zeta$$

[SG, M. E. Hochstenbach, *Probabilistic bounds for the matrix condition number with extended Lanczos bidiagonalization* (Submitted)]

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