Lecture 19: Conditioning of a problem

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1. Conditioning of a problem

- *Conditioning* pertains to the perturbation behavior of a mathematical *problem* $f : \mathbb{X} \to \mathbb{Y}$, where f is a function (explicitly or implicitly given, usually nonlinear, most of time at least continuous), and $\mathbb{X}$ and $\mathbb{Y}$ are normed vector spaces.
- A *problem* $f(x)$ is *well-conditioned* if all small perturbations of x lead to only small changes in $f(x)$; and is *ill-conditioned* if some small perturbation of x leads to a large change in $f(x)$.
- The *absolute condition number* of the problem $f(x)$ is defined as

$$\widehat{\kappa}(f(x)) = \lim_{\varepsilon \to 0^+} \sup_{\|\delta x\| \le \varepsilon} \frac{\|\delta f\|}{\|\delta x\|}, \quad \delta f = f(x + \delta x) - f(x).$$

- The *relative condition number* is defined by

$$\kappa(f(x)) = \lim_{\varepsilon \to 0^+} \sup_{\|\delta x\| \le \varepsilon} \left(\frac{\|\delta f\|}{\|f(x)\|} \Big/ \frac{\|\delta x\|}{\|x\|} \right).$$

2. Compute condition numbers

- If $f : \mathbb{X} \to \mathbb{Y}$ is differentiable, we can express $\widehat{\kappa}(f(x))$ and $\kappa(f(x))$ in terms of the Jacobian $\mathbf{J}(f(x))$, the matrix whose i, j entry is the partial derivative $\partial f_i / \partial x_j$ evaluated at x:

$$\widehat{\kappa}(f(x)) = \|\mathbf{J}(f(x))\|, \qquad \kappa(f(x)) = \frac{\|\mathbf{J}(f(x))\|}{\|f(x)\| / \|x\|},$$

  where $\|\mathbf{J}(f(x))\|$ represents the matrix norm of $\mathbf{J}(f(x))$ induced by the norms on $\mathbb{X}$ and $\mathbb{Y}$.

  Exercise: Prove $\widehat{\kappa}(f(x)) = \|\mathbf{J}(f(x))\|$ for all differentiable f.

  Example: For $f(x) = x/2$, we have

$$\kappa(f(x)) = 1.$$

  Example: For $f(x) = \sqrt{x}$ and $x > 0$, we have

$$\kappa(f(x)) = 1/2.$$

Example: Let $f(\mathbf{x}) = x_1 - x_2$ for $\mathbf{x} \in \mathbb{C}^2$ with the norm $\|\cdot\|_\infty$. The Jacobian of $f(\mathbf{x})$ is

$$\mathbf{J}(f(\mathbf{x})) = \begin{bmatrix} \partial_{x_1} f & \partial_{x_2} f \end{bmatrix} = \begin{bmatrix} 1 & -1 \end{bmatrix}.$$

By

$$\|\mathbf{J}(f(\mathbf{x}))\|_\infty = 2,$$

we obtain

$$\kappa(f(\mathbf{x})) = \frac{\|\mathbf{J}(f(\mathbf{x}))\|_\infty}{|f(\mathbf{x})|/\|\mathbf{x}\|_\infty} = \frac{2}{|x_1 - x_2|/\max\{|x_1|, |x_2|\}} = \frac{2\max\{|x_1|, |x_2|\}}{|x_1 - x_2|}.$$

This quantity is large if $|x_1 - x_2| \approx 0$, so the problem is ill-conditioned when $x_1 \approx x_2$.

This is the so called "cancellation error".

3. Polynomial rootfinding is typically ill-conditioned

- A simple case: assume that all roots are distinct and nonzero. Consider the polynomial

$$p(x) = \prod_{k=1}^{20}(x - x_k) = a_0 + a_1 x + \cdots + a_{19}x^{19} + x^{20}.$$

If only a_i is perturbed to $a_i + \delta a_i$, let $\widehat{x}_k$ denote the perturbed roots corresponding to x_k, then

$$\prod_{k=1}^{20}(x - \widehat{x}_k) - \prod_{k=1}^{20}(x - x_k) = (\delta a_i)x^i.$$

Therefore,

$$-\prod_{k=1}^{20}(\widehat{x}_j - x_k) = (\delta a_i)\widehat{x}_j^i.$$

By employing that x_j is a continuous function of a_i, we have

$$\begin{aligned}|(\delta x_j)p'(x_j)| &= |\widehat{x}_j - x_j| \prod_{k=1,k\neq j}^{20} |x_j - x_k| \\ &\sim \prod_{k=1}^{20} |\widehat{x}_j - x_k| = |(\delta a_i)\widehat{x}_j^i| \sim |(\delta a_i)x_j^i|.\end{aligned}$$

Therefore, the condition number of the problem $x_j = f(a_i)$ is

$$\kappa = \lim_{\varepsilon\to 0^+} \sup_{|\delta a_i|\leq\varepsilon} \frac{|\delta x_j|}{|x_j|} \Big/ \frac{|\delta a_i|}{|a_i|} = \frac{|a_i x_j^{i-1}|}{|p'(x_j)|}.$$

- Wilkinson polynomial:

$$p(x) = \prod_{k=1}^{20}(x-k) = a_0 + a_1 x + \cdots + a_{19}x^{19} + x^{20}.$$

We have $a_{15} \approx 1.67 \times 10^9$. For $x_{15} = 15$, we have

$$\kappa \approx \frac{1.67 \times 10^9 \times 15^{14}}{5!14!} \approx 5.1 \times 10^{13}.$$

4. Conditioning of matrix-vector multiplication

- For the problem $f_{\mathbf{A}}(\mathbf{x}) = \mathbf{A}\mathbf{x}$ where $\mathbf{A} \in \mathbb{C}^{m\times n}$, we have (by the definition)

$$\kappa(f_{\mathbf{A}}(\mathbf{x})) = \|\mathbf{A}\| \frac{\|\mathbf{x}\|}{\|\mathbf{A}\mathbf{x}\|}.$$

Exercise: Show the condition number of the problem $f_{\mathbf{x}}(\mathbf{A}) = \mathbf{A}\mathbf{x}$ is

$$\kappa(f_{\mathbf{x}}(\mathbf{A})) = \|\mathbf{x}\| \frac{\|\mathbf{A}\|}{\|\mathbf{A}\mathbf{x}\|}.$$

Discussion: What is the condition number of the problem

$$f(\mathbf{A}, \mathbf{x}) = \mathbf{A}\mathbf{x}$$

4.1. Interpolation sampling problem: $\mathbf{p} = \mathbf{A}\mathbf{f}$

- Let $x_1, \cdots, x_n$ be n distinct interpolation points and $y_1, \cdots, y_m$ be m sampling points from -1 to 1, respectively. The $m \times n$ matrix $\mathbf{A}$ that maps an n-vector of data $\{f(x_j)\}_{j=1}^{n}$ to an m-vector of sampled values $\{p(y_i)\}_{i=1}^{m}$, where p is the degree $n-1$ polynomial interpolant of $\{(x_j, f(x_j))\}_{j=1}^{n}$, is given by

$$\mathbf{A} = \mathbf{Y}\mathbf{X}^{-1},$$

where

$$\mathbf{X} = \begin{bmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^{n-1} \\ 1 & x_2 & x_2^2 & \cdots & x_2^{n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & \cdots & x_n^{n-1} \end{bmatrix}, \mathbf{Y} = \begin{bmatrix} 1 & y_1 & y_1^2 & \cdots & y_1^{n-1} \\ 1 & y_2 & y_2^2 & \cdots & y_2^{n-1} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & y_m & y_m^2 & \cdots & y_m^{n-1} \end{bmatrix}.$$

(a) Let $m = 2n - 1$. For equispaced points $\{x_j\}_{j=1}^n$ and $\{y_i\}_{i=1}^m$, the number $\|\mathbf{A}\|_\infty$ are known as the *Lebesgue constant* for equispaced interpolation, which is asymptotic to

$$2^n/(\mathrm{e}(n-1)\log n) \quad as \quad n \to \infty.$$

(b) By the condition number of matrix-vector multiplication,

$$\kappa = \|\mathbf{A}\|_\infty \frac{\|\mathbf{f}\|_\infty}{\|\mathbf{Af}\|_\infty},$$

we know some perturbation of $\mathbf{f}$ may lead to a large change in $\mathbf{p}$.
(c) For Chebyshev points ($j = 0 : n-1$, $i = 0 : m-1$),

$$x_j = \cos(j\pi/(n-1)), \quad y_i = \cos(i\pi/(m-1)).$$

Exercise: Compute $\|\mathbf{A}\|_\infty$ by Matlab and give your comments.

5. Condition number of a matrix

$$\kappa(\mathbf{A}) = \|\mathbf{A}\|\|\mathbf{A}^{-1}\|, \quad \text{or} \quad \kappa(\mathbf{A}) = \|\mathbf{A}\|\|\mathbf{A}^{\dagger}\|$$

6. Conditioning of a nonsingular system of equations $\mathbf{Ax} = \mathbf{b}$

- For the problem $g_{\mathbf{A}}(\mathbf{b}) = \mathbf{A}^{-1}\mathbf{b} \neq \mathbf{0}$ where $\mathbf{A} \in \mathbb{C}^{m\times m}$, we have

$$\kappa(g_{\mathbf{A}}(\mathbf{b})) = \|\mathbf{A}^{-1}\| \frac{\|\mathbf{b}\|}{\|\mathbf{A}^{-1}\mathbf{b}\|} \leq \|\mathbf{A}\|\|\mathbf{A}^{-1}\| = \kappa(\mathbf{A}).$$

- For the problem $g_{\mathbf{b}}(\mathbf{A}) = \mathbf{A}^{-1}\mathbf{b} \neq \mathbf{0}$, we have

$$\kappa(g_{\mathbf{b}}(\mathbf{A})) = \|\mathbf{A}\|\|\mathbf{A}^{-1}\| = \kappa(\mathbf{A}).$$

Proof. By dropping the doubly infinitesimal $(\delta\mathbf{A})(\delta\mathbf{x})$ from

$$(\mathbf{A} + \delta\mathbf{A})(\mathbf{x} + \delta\mathbf{x}) = \mathbf{b},$$

and using $\mathbf{Ax} = \mathbf{b}$, we have $(\delta\mathbf{A})\mathbf{x} + \mathbf{A}(\delta\mathbf{x}) = \mathbf{0}$, i.e.,

$$\delta \mathbf{x} = -\mathbf{A}^{-1}(\delta \mathbf{A})\mathbf{x} + o(\delta \mathbf{A}),$$

Therefore,

$$\|\delta \mathbf{x}\| = \|\mathbf{A}^{-1}(\delta \mathbf{A})\mathbf{x}\| + o(\|\delta \mathbf{A}\|) \leq \|\mathbf{A}^{-1}\|\|\delta \mathbf{A}\|\|\mathbf{x}\| + o(\|\delta \mathbf{A}\|),$$

and

$$\kappa(g_{\mathbf{b}}(\mathbf{A})) = \lim_{\varepsilon \to 0^+} \sup_{\|\delta \mathbf{A}\| \leq \varepsilon} \left(\frac{\|\delta \mathbf{x}\|}{\|\mathbf{x}\|} \Big/ \frac{\|\delta \mathbf{A}\|}{\|\mathbf{A}\|} \right) \leq \|\mathbf{A}\|\|\mathbf{A}^{-1}\|.$$

Now we begin to look for a special perturbation matrix $\delta \mathbf{A}$ which makes the upper bound attained. Let $\mathbf{z}$ be a vector to $\mathbf{x}$ such that (see the lemma in TreBau Exercise 3.6)

$$|\mathbf{x}^* \mathbf{z}| = \|\mathbf{z}\|' \|\mathbf{x}\|,$$

where $\|\cdot\|'$ denotes the *dual norm* defined by

$$\|\mathbf{z}\|' = \max_{\|\mathbf{y}\|=1} |\mathbf{y}^* \mathbf{z}|.$$

Let $\delta \mathbf{A} = \dfrac{\mathbf{u}\mathbf{z}^* \varepsilon}{\|\mathbf{z}\|'}$, where $\mathbf{u}$ is a unit vector ($\|\mathbf{u}\| = 1$) such that

$$\|\mathbf{A}^{-1}\mathbf{u}\| = \|\mathbf{A}^{-1}\|.$$

Obviously, $\|\delta \mathbf{A}\| = \varepsilon$ (verified by definition), and

$$\begin{aligned} \|\mathbf{A}^{-1}(\delta \mathbf{A})\mathbf{x}\| &= \frac{\varepsilon |\mathbf{z}^*\mathbf{x}|}{\|\mathbf{z}\|'} \|\mathbf{A}^{-1}\mathbf{u}\| \\ &= \varepsilon \|\mathbf{x}\| \|\mathbf{A}^{-1}\| \\ &= \|\mathbf{A}^{-1}\| \|\delta \mathbf{A}\| \|\mathbf{x}\|. \end{aligned}$$

Therefore, by

$$\|\delta \mathbf{x}\| = \|\mathbf{A}^{-1}(\delta \mathbf{A})\mathbf{x}\| + o(\|\delta \mathbf{A}\|) = \|\mathbf{A}^{-1}\| \|\delta \mathbf{A}\| \|\mathbf{x}\| + o(\|\delta \mathbf{A}\|),$$

we have

$$\kappa(g_{\mathbf{b}}(\mathbf{A})) = \lim_{\varepsilon \to 0^+} \sup_{\|\delta \mathbf{A}\| \le \varepsilon} \left(\frac{\|\delta \mathbf{x}\|}{\|\mathbf{x}\|} \Big/ \frac{\|\delta \mathbf{A}\|}{\|\mathbf{A}\|} \right) = \|\mathbf{A}\| \|\mathbf{A}^{-1}\|. \quad \square$$

7. Conditioning of least squares problems

- LSP: Given $\mathbf{A} \in \mathbb{C}^{m\times n}, m \geq n, \mathbf{b} \in \mathbb{C}^m$; find $\mathbf{x}_{\text{ls}} \in \mathbb{C}^n$ such that

$$\|\mathbf{b} - \mathbf{A}\mathbf{x}_{\text{ls}}\|_2 = \min_{\mathbf{x}\in\mathbb{C}^n} \|\mathbf{b} - \mathbf{A}\mathbf{x}\|_2.$$

- Assume that $\mathbf{A}$ is of full column rank. The unique least squares solution $\mathbf{x}_{\text{ls}}$ and the corresponding point $\mathbf{y} = \mathbf{A}\mathbf{x}_{\text{ls}}$ that is closest to $\mathbf{b}$ in range($\mathbf{A}$) are given by

$$\mathbf{x}_{\text{ls}} = \mathbf{A}^{\dagger}\mathbf{b} = (\mathbf{A}^*\mathbf{A})^{-1}\mathbf{A}^*\mathbf{b}, \quad \mathbf{y} = \mathbf{P}\mathbf{b} = \mathbf{A}\mathbf{x}_{\text{ls}},$$

  where $\mathbf{P} = \mathbf{A}\mathbf{A}^{\dagger}$ is the orthogonal projector onto range($\mathbf{A}$).

- Conditioning pertains to the sensitivity of solutions to perturbations in data.

$$\text{Data:} \quad \mathbf{A}, \mathbf{b} \qquad \text{Solutions:} \quad \mathbf{x}_{\text{ls}}, \mathbf{y}.$$

Theorem 1

Let $\mathbf{b} \in \mathbb{C}^m$ and $\mathbf{A} \in \mathbb{C}^{m \times n}$ of full column rank be fixed. The least squares problem has the following 2-norm relative condition numbers describing the sensitivities of $\mathbf{y}$ or $\mathbf{x}_{\text{ls}}$ to perturbations in $\mathbf{b}$ or $\mathbf{A}$:

	$\mathbf{y}$	$\mathbf{x}_{\text{ls}}$
$\mathbf{b}$	$\dfrac{1}{\cos\theta}$	$\dfrac{\kappa(\mathbf{A})}{\eta\cos\theta}$
$\mathbf{A}$	$\dfrac{\kappa(\mathbf{A})}{\cos\theta}$	$\kappa(\mathbf{A}) + \dfrac{\kappa(\mathbf{A})^2\tan\theta}{\eta}$

where

$$\theta = \arccos\frac{\|\mathbf{y}\|_2}{\|\mathbf{b}\|_2}, \quad \kappa(\mathbf{A}) = \|\mathbf{A}\|_2\|\mathbf{A}^\dagger\|_2, \quad \eta = \frac{\|\mathbf{A}\|_2\|\mathbf{x}_{\text{ls}}\|_2}{\|\mathbf{y}\|_2} = \frac{\|\mathbf{A}\|_2\|\mathbf{x}_{\text{ls}}\|_2}{\|\mathbf{A}\mathbf{x}_{\text{ls}}\|_2}.$$

The results in the second row are exact, being attained for certain perturbations $\delta\mathbf{b}$, and the results in the third row are upper bounds.

- Sensitivity of $\mathbf{y} = \mathbf{P}\mathbf{b} = \mathbf{A}\mathbf{A}^\dagger\mathbf{b}$ to perturbations in $\mathbf{b}$

$$\kappa_{\mathbf{b}\mapsto\mathbf{y}} = \|\mathbf{P}\|_2 \frac{\|\mathbf{b}\|_2}{\|\mathbf{y}\|_2} = \frac{1}{\cos\theta}$$

- Sensitivity of $\mathbf{x}_{\mathrm{ls}} = \mathbf{A}^\dagger\mathbf{b}$ to perturbations in $\mathbf{b}$

$$\kappa_{\mathbf{b}\mapsto\mathbf{x}_{\mathrm{ls}}} = \|\mathbf{A}^\dagger\|_2 \frac{\|\mathbf{b}\|_2}{\|\mathbf{x}_{\mathrm{ls}}\|_2} = \|\mathbf{A}^\dagger\|_2 \frac{\|\mathbf{b}\|_2}{\|\mathbf{y}\|_2} \frac{\|\mathbf{y}\|_2}{\|\mathbf{x}_{\mathrm{ls}}\|_2} = \frac{\kappa(\mathbf{A})}{\eta\cos\theta}$$

- Sensitivity of $\mathbf{x}_{\mathrm{ls}} = (\mathbf{A}^*\mathbf{A})^{-1}\mathbf{A}^*\mathbf{b}$ to perturbations in $\mathbf{A}$

$$\begin{aligned}\delta\mathbf{x}_{\mathrm{ls}} &= ((\mathbf{A}+\delta\mathbf{A})^*(\mathbf{A}+\delta\mathbf{A}))^{-1}(\mathbf{A}+\delta\mathbf{A})^*\mathbf{b} - \mathbf{x}_{\mathrm{ls}} \\ &= (\mathbf{A}^*\mathbf{A})^{-1}(\delta\mathbf{A})^*(\mathbf{I}-\mathbf{A}\mathbf{A}^\dagger)\mathbf{b} - \mathbf{A}^\dagger\delta\mathbf{A}\mathbf{A}^\dagger\mathbf{b} + o(\delta\mathbf{A})\end{aligned}$$

$$\kappa_{\mathbf{A}\mapsto\mathbf{x}_{\mathrm{ls}}} \le \frac{\|(\mathbf{I}-\mathbf{A}\mathbf{A}^\dagger)\mathbf{b}\|_2}{\sigma_n^2} \frac{\|\mathbf{A}\|_2}{\|\mathbf{x}_{\mathrm{ls}}\|_2} + \kappa(\mathbf{A}) = \frac{\kappa(\mathbf{A})^2\tan\theta}{\eta} + \kappa(\mathbf{A})$$

- Sensitivity of $\mathbf{y} = \mathbf{A}(\mathbf{A}^*\mathbf{A})^{-1}\mathbf{A}^*\mathbf{b}$ to perturbations in $\mathbf{A}$ (Exercise).

8. Computing the eigenvalues of a matrix

- If the matrix is *normal*, the problem is well-conditioned. We have (see Exercise 26.3)

$$\mathbf{A} \to \mathbf{A} + \delta\mathbf{A}, \quad \lambda \to \lambda + \delta\lambda : \quad |\delta\lambda| \le \|\delta\mathbf{A}\|_2.$$

Therefore, the absolute condition number is $\widehat{\kappa} = 1$, and the relative condition number is

$$\kappa = \frac{\|\mathbf{A}\|_2}{|\lambda|}.$$

- If the matrix is *nonnormal*, the problem is *often* ill-conditioned. For example,

$$\begin{bmatrix} 1 & 10^{16} \\ 0 & 1 \end{bmatrix}, \quad \begin{bmatrix} 1 & 10^{16} \\ 10^{-16} & 1 \end{bmatrix}$$

whose eigenvalues are $\{1, 1\}$ and $\{0, 2\}$, respectively.