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

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

• The relative condition number is defined by

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

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

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

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

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

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

If only a_i is perturbed to $a_i + \delta a_i$, let \hat{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

$$|(\delta x_j)p'(x_j)| = |\widehat{x}_j - x_j| \prod_{k=1, k \neq j}^{20} |x_j - x_k|$$

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

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

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

• Wilkinson polynomial:

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

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: p = Af

• Let x_1, \dots, x_n be n interpolation points and y_1, \dots, 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

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

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

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

we know some perturbation of f may lead to a large change in 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

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

- 6. Conditioning of a nonsingular system of equations Ax = 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

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

• 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 $\mathbf{A}\mathbf{x} = \mathbf{b}$, 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,

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

and

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

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 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 $\delta \mathbf{A} = \frac{\mathbf{u}\mathbf{z}^* \varepsilon}{\|\mathbf{z}\|'}$, 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

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

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

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

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 $\mathbf{x}_{ls} \in \mathbb{C}^n$ such that

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

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

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

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.

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

Theorem 1

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

$$\begin{array}{ccc} & \mathbf{y} & \mathbf{x}_{\mathrm{ls}} \\ \mathbf{b} & \frac{1}{\cos \theta} & \frac{\kappa(\mathbf{A})}{\eta \cos \theta} \\ \mathbf{A} & \frac{\kappa(\mathbf{A})}{\cos \theta} & \kappa(\mathbf{A}) + \frac{\kappa(\mathbf{A})^2 \tan \theta}{\eta} \end{array}$$

where

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

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

$$\kappa_{\mathbf{b} \mapsto \mathbf{x}_{ls}} = \|\mathbf{A}^{\dagger}\|_{2} \frac{\|\mathbf{b}\|_{2}}{\|\mathbf{x}_{ls}\|_{2}} = \|\mathbf{A}^{\dagger}\|_{2} \frac{\|\mathbf{b}\|_{2}}{\|\mathbf{y}\|_{2}} \frac{\|\mathbf{y}\|_{2}}{\|\mathbf{x}_{ls}\|_{2}} = \frac{\kappa(\mathbf{A})}{\eta \cos \theta}$$

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

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

$$\kappa_{\mathbf{A} \mapsto \mathbf{x}_{ls}} \leq \frac{\|(\mathbf{I} - \mathbf{A} \mathbf{A}^{\dagger}) \mathbf{b}\|_{2}}{\sigma_{n}^{2}} \frac{\|\mathbf{A}\|_{2}}{\|\mathbf{x}_{ls}\|_{2}} + \kappa(\mathbf{A}) = \frac{\kappa(\mathbf{A})^{2} \tan \theta}{\eta} + \kappa(\mathbf{A})$$

• Sensitivity of $\mathbf{y} = \mathbf{A}(\mathbf{A}^*\mathbf{A})^{-1}\mathbf{A}^*\mathbf{b}$ to perturbations in \mathbf{A} . Exercise. Prove the upper bound in Theorem 1 for $\kappa_{\mathbf{A}\mapsto\mathbf{y}}$.

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 $\hat{\kappa} = 1$, 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,

$$\left[\begin{array}{cc} 1 & 10^{16} \\ 0 & 1 \end{array}\right], \quad \left[\begin{array}{cc} 1 & 10^{16} \\ 10^{-16} & 1 \end{array}\right]$$

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