LECTURE 13

CONDITION NUMBER

Measures the sensivity of a problem to perturbations (for instance to rounding errors)

$$f : V \longrightarrow W$$

f is a function from a vector space V to another vector space W.

EXAMPLES

① Consider

$$p_\epsilon(x) = x^2 - \epsilon$$

Positive root as a function of ϵ

$$r_+(\epsilon) : \mathbb{R} \longrightarrow \mathbb{C}$$

$$r_+(\epsilon) = \sqrt{\epsilon}$$

(2)

$$f : \mathbb{R}^2 \longrightarrow \mathbb{R}$$

$$f(x) = x_1^2 - x_2^2$$

(3) Given $A \in \mathbb{C}^{n \times n}$ and $b \in \mathbb{C}^n$.
Consider the linear system

$$Ax = b$$

The solution x as a function of A.

$$x : \mathbb{C}^{n \times n} \longrightarrow \mathbb{C}^n \quad \text{(assume } b \text{ is fixed)}$$

$$x(A) = A^{-1}b \quad \text{(assuming } A \text{ is invertible)}$$

(4) Least squares problem

Given $A \in \mathbb{C}^{m \times n}$ (with $m > n$)
and $b \in \mathbb{C}^m$. Find $\hat{x}$ so that

$$\| A\hat{x} - b \|_2$$

is as small as possible.

The solution $\hat{x}$ as a function of b

$$\hat{x} : \mathbb{C}^n \longrightarrow \mathbb{C}^m$$

$$\hat{x}(b) = (A^* A)^{-1} A^* b \quad \text{(assuming rank}(A) = n\text{; follows from the normal eqn)}$$

Sensitivity of f

How does f change w.r.t. changes in the input?

Absolute Condition Number

Measure of sensitivity of $f(x)$

$$\kappa = \lim_{\delta \to 0} \sup_{\|\delta x\| \leq \delta} \frac{\|\overbrace{f(x+\delta x)-f(x)}^{\delta f}\|}{\|\delta x\|}$$

EXAMPLE

Positive root of $p_\epsilon(x) = x^2 - \epsilon$ as a function of ϵ at $\epsilon = 0$

$$\frac{|\overbrace{r_+(\delta\epsilon) - r_+(0)}^{\delta r_+}|}{|\delta\epsilon|} \doteq \frac{|\sqrt{\delta\epsilon} - 0|}{|\delta\epsilon|}$$

$$= \frac{1}{|\sqrt{\delta\epsilon}|}$$

$$\kappa = \lim_{\delta \to 0} \sup_{|\delta\epsilon| \leq \delta} \frac{1}{|\sqrt{\delta\epsilon}|}$$

$$= \infty$$

Root-finding problem in general is ill-conditioned.

TERMINOLOGY

ill-conditioned : condition number is large

well-conditioned : condition number is small

REMINDER

sup S : supremum (smallest upper bound) of the set S.

e.g.

$$\sup\left\{\frac{1}{n} : n > 1\right\} = 1$$

$$\sup\left\{\frac{x^2-1}{2x^2} : x \neq 0\right\} = \frac{1}{2}$$

Jacobian of a multi-variate function

$$f : \mathbb{C}^n \longrightarrow \mathbb{C}^m$$

$$\boxed{\text{Jacobian of } f \text{ at } x} \quad J(x) = \begin{bmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} & \cdots & \frac{\partial f_1}{\partial x_n} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} & \cdots & \frac{\partial f_2}{\partial x_n} \\ \vdots & & & \\ \frac{\partial f_m}{\partial x_1} & \frac{\partial f_m}{\partial x_2} & \cdots & \frac{\partial f_m}{\partial x_n} \end{bmatrix}_{m \times n} \quad \left(\text{matrix of partial derivatives}\right)$$

EXAMPLES

① $f(x) = x_1^2 - x_2^2$

$$J(x) = \begin{bmatrix} 2x_1 & -2x_2 \end{bmatrix}$$

② $f(x) = \begin{bmatrix} x_1^2 - x_2^2 \\ x_1 x_2 \end{bmatrix}$

$$J(x) = \begin{bmatrix} 2x_1 & -2x_2 \\ x_2 & x_1 \end{bmatrix}$$

REMARK

Suppose $f : \mathbb{C}^n \to \mathbb{C}$

$$J(x) = \begin{bmatrix} \frac{\partial f}{\partial x_1} & \frac{\partial f}{\partial x_2} & \cdots & \frac{\partial f}{\partial x_n} \end{bmatrix}$$

$$= \nabla f(x)^T$$

where $\nabla f(x)$ is the gradient vector

$$\nabla f(x) = \begin{bmatrix} \partial f/\partial x_1 \\ \partial f/\partial x_2 \\ \vdots \\ \partial f/\partial x_n \end{bmatrix}$$

Absolute condition number in terms of Jacobian

Suppose $f: \mathbb{C}^n \to \mathbb{C}^m$ is twice differentiable. Then (by Taylor's thm; we will see this in detail next semester)

$$(*) \quad f(x+\delta x) = f(x) + J(x)\,\delta x + O(\|\delta x\|^2)$$

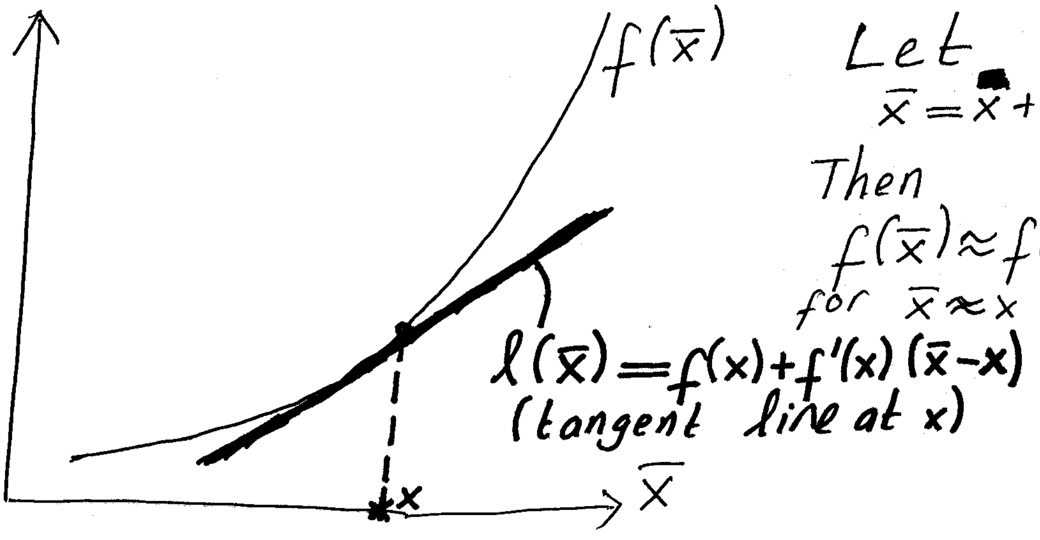
REMARKS

(1) We are interested in δx small in norm. $O(\|\delta x\|^2)$ represents terms proportional to $\|\delta x\|^2$ or smaller (e.g. $2\|\delta x\|^2 + \|\delta x\|^3$); This is the usual big-O notation, but we take the limit as $\delta x \to 0$. $g(\delta x) = O(f(\delta x))$ means $cf(\delta x)$ dominates $g(\delta x)$ as $\delta x \to 0$ for some constant c.

(2) Suppose $f: \mathbb{R} \to \mathbb{R}$ is differentiable. Then

$$f(x+\delta x) \approx f(x) + f'(x)\,\delta x$$

is the linear (tangent line) approximation at x.



Let $\bar{x} = x + \delta x$.

Then $f(\bar{x}) \approx f(x) + f'(x)(\bar{x}-x$

for $\bar{x} \approx x$

More generally when $f: \mathbb{C}^n \to \mathbb{C}^m$

$$f(x+\delta x) \approx f(x) + J(x)\,\delta x$$

is the linear approximation at x.

Using (*)

$$\kappa = \lim_{\delta \to 0} \sup_{\|\delta x\| \leq \delta} \frac{\|f(x+\delta x) - f(x)\|}{\|\delta x\|}$$

$$= \lim_{\delta \to 0} \sup_{\|\delta x\| \leq \delta} \frac{\|f(x) + J(x)\delta x + O(\|\delta x\|^2) - f(x)\|}{\|\delta x\|}$$

$$= \lim_{\delta \to 0} \sup_{\|\delta x\| \leq \delta} \frac{\|J(x)\,\delta x\| + O(\|\delta x\|^2)}{\|\delta x\|}$$

$$= \cancel{\lim_{\delta \to 0}} \|J(x)\| = \underbrace{\|J(x)\|}_{\text{vector induced matrix norm}}$$

SUMMARY

For $f: \mathbb{C}^n \to \mathbb{C}^m$ twice differentiable

$$\boxed{\kappa = \|J(x)\|}$$

EXAMPLE

For $f(x) = x_1^2 - x_2^2$ using the 2-norm

$$\kappa = \|[2x_1 \ \ -2x_2]\|_2 = 2\|x\|_2$$

Relaxed absolute condition number

For $\delta > 0$ small in absolute value

$$K_\delta = \sup_{\|\delta x\| \leq \delta} \frac{\|f(x+\delta x) - f(x)\|}{\|\delta x\|}$$

For small δ

$$K \approx K_\delta$$

We will often depend on K_δ rather than K in our accuracy analyses.

EXAMPLE

Matrix-vector product as a function of matrix

$$f : \mathbb{C}^{n \times n} \longrightarrow \mathbb{C}^n$$

$$f(A) = Ax \quad (x \text{ is fixed})$$

Then

$$K_\delta = \sup_{\|\delta A\| \leq \delta} \frac{\|f(A+\delta A) - f(A)\|}{\|\delta A\|}$$

$$= \sup_{\|\delta A\| \leq \delta} \frac{\|(A+\delta A)x - Ax\|}{\|\delta A\|}$$

$$= \sup_{\|\delta A\| \leq \delta} \frac{\|\delta A\, x\|}{\|\delta A\|}$$

$$= \sup_{\|\delta A\| \leq \delta} \frac{\|\delta A\| \, \|x\|}{\|\delta A\|} = \|x\|$$

Choose δA s.t.
$\|\delta A x\| = \|\delta A\| \, \|x\|$

Indeed

$$\kappa = \lim_{\delta \to 0} \kappa_\delta = \|x\|$$

<u>Relative condition number</u>

$$\tilde{\kappa} = \lim_{\delta \to 0} \sup_{\|\delta x\| \leq \delta} \frac{\|f(x+\delta x) - f(x)\| / \|f(x)\|}{\|\delta x\| / \|x\|}$$

$$= \frac{\kappa \, \|x\|}{\|f(x)\|}$$

Relative condition number is used more often than the absolute condition number in practice. This is due to fact that IEEE standards introduce constant relative errors (proportional to ϵ_{mach}).

<u>EXAMPLE</u>

For $f(x) = x_1^2 - x_2^2$ using the 2-norm

$$\tilde{\kappa} = \frac{\|[2x_1 \;\; -2x_2]\|_2 \, \|x\|_2}{|x_1^2 - x_2^2|}$$

$$\tilde{\kappa} = 2\|x\|_2^2 / |x_1^2 - x_2^2|$$

$\tilde{\kappa}$ is large (problem is ill-conditioned) if $x_1 \approx x_2$.

For $f : \mathbb{C}^n \longrightarrow \mathbb{C}^m$ twice-differentiable

$$\tilde{\kappa} = \frac{\|J(x)\| \, \|x\|}{\|f(x)\|}$$

Relaxed relative condition number

$$\tilde{\kappa}_\delta = \sup_{\|\delta x\| \leqslant \delta} \frac{\|f(x+\delta x) - f(x)\| / \|f(x)\|}{\|\delta x\| / \|x\|}$$

$$= \frac{\kappa_\delta \, \|x\|}{\|f(x)\|}$$

where $\delta > 0$ (supposed to be small in absolute value)

For small $\delta > 0$

$$\tilde{\kappa} \approx \tilde{\kappa}_\delta$$

EXAMPLE

For the matrix-vector product example with

$$f(A) = Ax$$

we have

$$\tilde{\kappa}_\delta = \frac{\kappa_\delta \|A\|}{\|f(A)\|} = \frac{\|x\| \, \|A\|}{\|Ax\|}.$$

Notice that (assuming A is invertible)

$$\|x\| = \|A^{-1}Ax\| \leqslant \|A^{-1}\| \, \|Ax\|$$

$$\Longrightarrow$$

$$\frac{\|x\|}{\|Ax\|} \leqslant \|A^{-1}\|$$

Therefore

$$\tilde{\kappa}_\delta \leqslant \|A^{-1}\| \, \|A\|$$

and

$$\tilde{\kappa} = \lim_{\delta \to 0} \tilde{\kappa}_\delta \leqslant \|A^{-1}\| \, \|A\|$$

Condition number of a matrix

The quantity

$$\kappa(A) = \|A\| \, \|A^{-1}\|$$

occurs so often in accuracy analyses that it is called the condition number of A.

EXAMPLE

Let

$$A = \begin{bmatrix} 3 & 0 \\ 0 & 1 \end{bmatrix}$$

and

$$A^{-1} = \begin{bmatrix} 1/3 & 0 \\ 0 & 1 \end{bmatrix}$$

Condition number of A w.r.t. the 2-norm

$$\kappa(A) = \|A\|_2 \, \|A^{-1}\|_2$$

$$= 3 \cdot 1 = 3$$

Condition number of a matrix w.r.t. 2-norm

Let

$$A = U \Sigma V^*$$

be an SVD of $A \in \mathbb{C}^{n \times n}$.

Then an SVD for A^{-1} is given by

$$A^{-1} = (V^*)^{-1} \Sigma^{-1} U^{-1}$$

$$= V \Sigma^{-1} U^*.$$

In particular suppose

$$\Sigma = \begin{bmatrix} \sigma_1 & & & 0 \\ & \sigma_2 & & \\ & & \ddots & \\ 0 & & & \sigma_n \end{bmatrix} \quad \left(\begin{matrix} \text{where} \\ \sigma_1 \geq \sigma_2 \geq \cdots \geq \sigma_n \end{matrix} \right)$$

meaning

$$\Sigma^{-1} = \begin{bmatrix} 1/\sigma_1 & & & 0 \\ & 1/\sigma_2 & & \\ & & \ddots & \\ 0 & & & 1/\sigma_n \end{bmatrix} \Longrightarrow \|A^{-1}\|_2 = \|\Sigma^{-1}\|_2 = 1/\sigma_n$$

Condition number of A in terms of singular values

$$\kappa(A) = \|A\|_2 \, \|A^{-1}\|_2 = \frac{\sigma_1}{\sigma_n}$$