Part 2: Condition Numbers

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0.1 Root-finding

Last time, we described a geometric proof of the fundamental theorem of algebra. The rough idea was this: we identify a polynomial with a point in Euclidean space

$$f(x) := a_d x^d + \ldots + a_0 \quad \Leftrightarrow \quad (a_d, \ldots, a_0) \in \mathbb{C}^{d+1}.$$

Then, we try to understand a "function" from $\mathbb{C}^{d+1}$ to $\mathbb{C}$ that sends f to one of its roots. Of course, this function cannot be globally well-defined, since polynomials generally have more than one root! So, suppose we are given a polynomial $f \in U \subset \mathbb{C}^{d+1}$, where U is an open set. To be able to solve for a unique root, we'll need the implicit function theorem like in the last lecture. So, assume further that $f \notin \Sigma_d$, the degenerate set from the last lecture. Shrinking U further if necessary, we may assume $U \cap \Sigma_d = \emptyset$.

By the implicit function theorem, there exists a solution function $Z : U \to \mathbb{C}$ that sends any $g \in U$ to a unique root $Z(g)$. In fact, we have a recipe for differentiating this solution function. Let's consider any homotopy function $H(x;t)$ with the property $H(x;0) = f(x)$. For t with $H(x;t) \in U$, we write $z(t) = Z\left(H(x;t)\right)$.

Now, for t sufficiently small, we have

$$H(z(t);t) = 0 \quad \Rightarrow \quad \frac{dH}{dx}(z(t);t) \cdot z'(t) + \frac{dH}{dt}(z(t);t) = 0 \quad \Rightarrow \quad z'(t) = -\left(\frac{dH}{dx}(z(t);t)\right)^{-1} \cdot \frac{dH}{dt}(z(t);t).$$

Let $r = z(0)$ denote the local root of f. Evaluating the above at $t = 0$, we obtain

$$z'(0) = -\left(f'(r)\right)^{-1} \cdot \frac{dH}{dt}(r;0) \tag{1}$$

Equation (1) will help us understand the *condition number* for the polynomial root finding problem. This is a quantity that tells us how sensitive our root-finding function is to "small" perturbations in the coefficients of the input. To define "small" more precisely, let us endow the input space $\mathbb{C}^{d+1}$ with the usual Hermitian inner product and norm. For $\vec{a} = (a_d, \ldots, a_0)$, $\vec{b} = (b_d, \ldots, b_0) \in \mathbb{C}^{d+1}$, we define

$$\langle \vec{a}, \vec{b} \rangle = \sum_{j=0}^{d} a_i \bar{b}_i$$
$$\|\vec{a}\| = \sqrt{\langle \vec{a}, \vec{a} \rangle}.$$

Here, $\bar{\zeta}$ denotes the usual complex conjugate of $\zeta \in \mathbb{C}$. We recall the *Cauchy-Schwartz inequality:*

$$|\langle \vec{a}, \vec{b} \rangle|^2 \le \|\vec{a}\|^2 \|\vec{b}\|^2,$$

where $\|\zeta\| = \sqrt{\zeta\bar{\zeta}}$ is the usual modulus. This has the following geometric consequence: for fixed $\vec{a} \in \mathbb{C}^{d+1}$,

$$\max_{\|\vec{b}\|=1} |\langle \vec{a}, \vec{b} \rangle| = \|\vec{a}\|. \tag{2}$$

Let us again examine equation 1: we have

$$\begin{aligned} z'(0) &= -\left(f'(r)\right)^{-1} \langle \vec{r}, \vec{c} \rangle, \text{ where} \\ \vec{r} &= (r^d, \ldots, 1), \\ \vec{c} &= (c_d, \ldots, c_0), \text{ and} \\ \frac{dH}{dt}(x;0) &= \bar{c}_d x^d + \ldots + \bar{c}_0. \end{aligned}$$

This expresses the derivative of the solution function at f as the linear map

$$\begin{aligned}Z'(f) : \mathbb{C}^{d+1} &\to \mathbb{C}\\ \vec{c} &\mapsto -\left(f'(r)\right)^{-1}\langle \vec{r}, \vec{c}\rangle\end{aligned}$$

For those familiar with tangent spaces (which we'll come back and define later): this map "pushes forward" a tangent vector $\vec{c} \in \mathbb{C}^{d+1} \cong T_f(\mathbb{C}^{d+1})$ into $\mathbb{C} \cong T_r(\mathbb{C})$. Now, if $g = \bar{c}_d x^d + \ldots + \bar{c}_0$ is a small perturbation of f, then

$$|Z(f) - Z(g)| \approx \|Z'(f)\|_{op} \cdot \|f - g\|,$$

where $\| \bullet \|_{op}$ denotes the *operator norm*,

$$\begin{aligned}\|Z'(f)\|_{op} &= \max_{\|\vec{c}\|=1} |Z'(f) \cdot \vec{c}| && (3)\\ &= |f'(r)|^{-1} \cdot \sqrt{\sum_{j=0}^{d} |r|^{2j}} && \text{(by 2.)}\end{aligned}$$

Thus, the amount by which a root r of a polynomial of f varies when the coefficients of f are slightly perturbed can be quantified in terms of f and r alone. This quantity is an example of a condition number.

Definition 0.1. Let $f = a_d x^d + \ldots + a_0$ be a univariate polynomial of degree d with a non-repeated root r. The *absolute condition number* of root-finding for f at r (with respect to the usual Hermitian norm) is the number

$$\kappa[r](f) = |f'(r)|^{-1} \cdot \sqrt{\sum_{j=0}^{d} |r|^{2j}}. \tag{4}$$

Remark 0.2. Clearly the assumption that r is non-repeated in Definition 0.1 is necessary. Note also that this definition could also be modified by choosing different norms on the input space $\mathbb{C}^{d+1}$ and the output space $\mathbb{C}$.

Now, in numerical analysis, we are usually interested in controlling *relative errors* like

$$\||f - g\||/\|f\|, \quad |Z(f) - Z(g)|/|Z(f)|.$$

In other words: what is computed should not differ from the true values by a significant percentage of the "size" of those true values. This motivates the following definition.

Definition 0.3. With the same setup as Definition 0.1, we define the *relative condition number* to be

$$\kappa_{\text{REL}}[r](f) = \frac{\|f\| \, \kappa[r](f)}{|r|} = |r f'(r)|^{-1} \cdot \sqrt{\sum_{j=0}^{d} |r|^{2j}} \cdot \sqrt{\sum_{j=0}^{d} |a_j|^2}. \tag{5}$$

Example 1. A famous example of a poorly-conditioned polynomial is *Wilskinson's polynomial*

$$f(x) = (x - 1) \cdot (x - 2) \cdots (x - 20).$$

The perturbed polynomial $f + 10^{-10} x^{19}$ has roots given approximately by

$1, \ldots, 7, 7.99994, 9.00084, 9.99252, 11.0506, 11.8329, 13.349, 13.349, 15.4578, 15.4578, 17.6624, 17.6624, 19.2337, 19.9509.$

The perturbed polynomial $f + 10^{-9} x^{19}$ has multiple non-real roots. We see that the small roots of f are fairly well-conditioned: for instance, we may calculate

$$\kappa[1](f) \approx 10^{-16}, \quad \kappa_{\text{REL}}[1](f) \approx 857.$$

For the larger roots, the situation is much more dire: for example,

$$\kappa[15](f) \approx 3.8 \times 10^{10}, \quad \kappa_{\text{REL}}[15](f) \approx 5.4 \times 10^{28}.$$

This example is counter-intuitive because the polynomial is "given" in a simple way (factored). However, the condition numbers we defined assume the polynomial is "given" by its coefficients, which are enormous.

0.2 Linear Algebra

Moving on from polynomial root-finding for now, let's look at condition numbers for the more classical problem of matrix inversion. This was the original context in which condition numbers were introduced by Turing.

For the time being, we will work with the space $\mathbb{R}^{m\times n}$ whose points are real $m \times n$ matrices. This is a vector space which can be endowed with many norms. We will mostly think about the *Euclidean/Frobenius norm*

$$\|A\| = \sqrt{\operatorname{trace}(A^T A)} = \sqrt{\sum_{\substack{1\le i\le m\\ 1\le j\le n}} a_{ij}^2}, \tag{6}$$

and the associated operator norm, commonly known as the *spectral norm*,

$$\|A\|_{op} = \max_{\|x\|=1} \|Ax\|. \tag{7}$$

Both norms are *orthogonally invariant*: if $U \in \mathbb{R}^{m\times m}$ and $V \in \mathbb{R}^{n\times n}$ are both orthogonal matrices, then we have

$$\|UAV\| = \|A\|, \quad \|UAV\|_{op} = \|A\|_{op}.$$

Thus, both norms can be expressed in terms of the *singular value decomposition* (in fact, the *singular values*) of A: if $A = U\Sigma V^T$, with U and V orthogonal and Σ with non-zero entries $\sigma_1 \ge \ldots \ge \sigma_r > 0$ on the main diagonal, then

$$\|A\| = \sigma_1^2 + \ldots + \sigma_r^2, \quad \|A\|_{op} = \sigma_1.$$

Here is an important property of the operator norm:

Proposition 0.4. For $A \in \mathbb{R}^{m\times n}, B \in \mathbb{R}^{n\times k}$, we have $\|AB\|_{\mathrm{op}} \le \|A\|_{\mathrm{op}} \|B\|_{\mathrm{op}}$.

Proof.

$$\begin{aligned}
\|AB\|_{op} &= \max_{\|x\|=1} \|(AB)x\| \\
&= \max_{x\neq 0} \frac{\|(AB)x\|}{\|x\|} \\
&= \max_{x\neq 0} \left(\frac{\|A(Bx)\|}{\|Bx\|} \cdot \frac{\|Bx\|}{\|x\|} \right) \\
&\le \max_{x,y\neq 0} \left(\frac{\|Ay\|}{\|y\|} \cdot \frac{\|Bx\|}{\|x\|} \right) = \|A\|_{op} \|B\|_{op}.
\end{aligned}$$

□

We now study the derivative of the map $\operatorname{inv} : U \to U$ at a point $A \in U$, where $U \subset \mathbb{R}^{n\times n}$ is the open set of all invertible matrices. Again, implicit differentiation comes to the rescue:

$$AB = I \quad \Rightarrow \quad \dot{A}B + A\dot{B} = 0 \quad \Rightarrow \quad \dot{B} = -A^{-1}\dot{A}B = -A^{-1}\dot{A}A^{-1}.$$

This expresses the derivative of inv at the point A as a linear map between tangent spaces,

$$\dot{\operatorname{inv}}_A : \overbrace{\mathbb{R}^{n\times n}}^{\cong T_A(U)} \to \overbrace{\mathbb{R}^{n\times n}}^{\cong T_{A^{-1}}(\mathbb{R}^{n\times n})}$$
$$\dot{A} \mapsto -A^{-1}\dot{A}A^{-1}.$$

Let us now endow both the input space U and the output space $\mathbb{R}^{n\times n}$ with the operator norm. With respect to these choices, we may use orthogonal invariance and Proposition 0.4 to compute the operator norm of the derivative,

$$\max_{\|\dot{A}\|_{op}=1} \|\dot{\operatorname{inv}}_A(\dot{A})\|_{op} = \max_{\|\dot{A}\|_{op}=1} \|A^{-1}\dot{A}A^{-1}\|_{op} = \max_{\|\dot{A}\|_{op}=1} \|\Sigma^{-1}\dot{A}\Sigma^{-1}\|_{op} \le \|\Sigma^{-1}\|_{op}^2,$$

with equality attained when $\dot{A} = I$. Thus

$$\max_{\|\dot{A}\|_{op}=1} \|\dot{\operatorname{inv}}_A(\dot{A})\|_{op} = \|\Sigma^{-1}\|_{op}^2 = \|A^{-1}\|_{op}^2 = 1/\sigma_n^2.$$

This calculation justifies the following definition.

Definition 0.5. Let A be a nonsingular matrix with greatest singular value σ_1 and least singular value σ_n. The absolute and relative condition numbers of matrix inversion at A are given by

$$\kappa[\text{inv}](A) = \frac{1}{\sigma_n^2}, \quad \kappa_{\text{REL}}[\text{inv}] = \frac{\|A\|_{op}\, \kappa[\text{inv}](A)}{\|A^{-1}\|_{op}} = \frac{\sigma_1}{\sigma_n}. \tag{8}$$

Remark: Suppose we endowed our input and output spaces with the Frobenius norm instead of the operator norm. How would the condition numbers in Definition 0.5 change? It turns out that the absolute condition number does not change: working with the square operator norm of the derivative, we have

$$\max_{\|\dot{A}\|=1} \|\dot{\text{inv}}_A(\dot{A})\|^2 = \max_{\|\dot{A}\|=1} \|A^{-1}\dot{A}A^{-1}\|_{op}^2 = \max_{\|\dot{A}\|=1} \|\Sigma^{-1}\dot{A}\Sigma^{-1}\|^2 = \max_{\sum \dot{a}_{i,j}^2=1} \sum_{1\le i,j\le n} \frac{\dot{a}_{i,j}^2}{\sigma_i^2\,\sigma_j^2}.$$

Using $\sigma_i\sigma_j \geq \sigma_n^2$, we have

$$\max_{\|\dot{A}\|=1} \|\dot{\text{inv}}_A(\dot{A})\|^2 \leq \frac{1}{\sigma_n^4}\,,$$

with equality attained when $\dot{a}_{n,n} = 1$ and all other entries are zero. Taking the square root gives us the absolute condition number

$$\max_{\|\dot{A}\|=1} \|A^{-1}\dot{A}A^{-1}\| = \frac{1}{\sigma_n^2}.$$

The relative condition number, on the other hand, becomes more unwiedly:

$$\frac{1}{\sigma_n^2} \cdot \frac{\|A\|}{\|A^{-1}\|} = \frac{1}{\sigma_n^2}\sqrt{\frac{\sigma_1^2 + \ldots + \sigma_n^2}{\sigma_1^{-2} + \ldots + \sigma_n^{-2}}}.$$

Next steps: Just like the case of polynomial root-finding, there is a set of degenerate instances for the problem of inverting a matrix. This set is defined by the equation $\det A = 0$. Amazingly, the *Eckart-Young Theorem* states that $1/\kappa[\text{inv}](A)$ can be interpreted as the squared distance from A to this set. This is a special instance of a cornerstone problem in applied algebraic geometry: namely, minimizing the Euclidean distance from a point $u \in \mathbb{R}^n$ to a real algebraic variety $X \subset \mathbb{R}^n$. This will be the focus of the next lecture.

Reference: Breiding, P, Kohn, K, and Sturmfels, B (2024). Metric Algebraic Geometry (Chapter 9).