14. Conditioning of a problem and stability of an algorithm

Summary of the previous class

- The Singular-Value Decomposition (SVD)
  - $\mathsf{A} = \mathsf{U}\Sigma\mathsf{V}^\mathsf{T}$
- Calculation via eigen-decomposition of symmetric matrix
  - $\mathsf{A}\mathsf{A}^\mathsf{T}$
- Application to understanding and compressing data
- PCA and best-fitting k-dimensional subspace

Goals for today's class

- **Conditioning**: How sensitive is a **problem**

- Catastrophic cancellation
- **Stability** of an **algorithm**

Conditioning of a problem

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- Example: Intersection of two thick lines at an angle

Collaboration I

Perturbing input and output

1. What is the relationship between Δx and Δy?
2. What does the form of the resulting equation suggest?
3. What might be a better way of measuring the perturbation in x?

Absolute errors

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- Δx and Δy are **absolute errors**

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- So $\hat{x} = x + \Delta x = x(1 + \delta x)$
- And $\hat{y} = y + \Delta y = y(1 + \delta y)$

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- We can express this in terms of the number of **significant** or **accurate digits**:

$$d = -\log_{10} |\delta x|$$

- This gives the number of digits after which $\hat{x}$ and x differ
- Independently of the absolute size of x

Collaboration II

1. Calculate the number of accurate digits for the approximation $22/7$ of π
2. Does that make sense?
3. How could you get better approximations?

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- How can we **measure** the conditioning of a *problem*?

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- In face we need $\hat{\kappa}_\phi(x, \epsilon)$, taking the maximum over inputs with $\|\Delta x\| < \epsilon$

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- Provided ϕ is differentiable

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Collaboration III

Condition number of addition

Addition of two numbers is a very basic operation in numerical computing. We hope that it is well-conditioned. Is it?

1. Calculate the absolute condition number for the problem $\phi(x) = x + a$ with a fixed a.
2. Calculate the relative condition number for addition.
3. Can the relative condition number be large?

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$$= a + (x + \Delta x) - (a + x) = \Delta x$$

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- But we really care about the *relative* condition number

Condition number of addition II

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- Note that $\phi(x)$ appears in the *denominator*
- So κ_ϕ is *large* when $x \simeq -a$
- **Catastrophic cancellation**: Loss of accuracy when *subtracting* two numbers that are close
- Common task: **identify** + **eliminate** catastrophic cancellation

Collaboration IV

Quadratic equations

1. Formulate “solving a quadratic equation” as a problem. What are the inputs and outputs?
2. What can go wrong?

Quadratic equations

- Let's look at solving a quadratic equation $ax^2 + bx + c = 0$
- What is the problem ϕ?
- The input $\mathcal{X}$ is (a, b, c)
- The output $\mathcal{Y}$ is the set of two roots $x_\pm$ given by

$$x_\pm = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

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- If $b > 0$ and ac is small, then x_+ has catastrophic cancellation

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- Problem: $\Phi(a) = x_+(a)$ (with b and c fixed)

- Suppose we move a to $a + \Delta a$
- Then the root x_+ moves to $x_+ + \Delta x_+$

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- So the condition number is *large* when the roots are *close*
- We can visualize this by perturbing the quadratic function

Conditioning for linear systems

Norms

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- For vectors $\mathbf{v} \in \mathbb{R}^m$ we will use the 2-norm:

$$\|\mathbf{v}\|_2 := \sqrt{\sum_{i=1}^{m} v_i^2}$$

Induced matrix norm

- There are various ways of measuring the size (norm) of a matrix that are useful for different purposes
- We will use the matrix norm **induced** from a given vector norm

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- Suppose A is a square $(m \times m)$ matrix
- For each **x** we can measure $\|\mathbf{x}\|$ and $\|\mathsf{A}\mathbf{x}\|$ . . .
- We define the induced matrix norm as the smallest C such that

$$\|\mathsf{A}\| \leq C\|\mathbf{x}\| \quad \forall \mathbf{x} \in \mathbb{R}^m$$

Induced matrix norm II

- Hence

$$\|A\| = \sup_{\|\mathbf{x}\|=1} \|A\mathbf{x}\|$$

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- Note that $\|A\mathbf{x}\| \leq \|A\|\|\mathbf{x}\|$

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- Simplest case: Perturb the input $\mathbf{b}$ to $\mathbf{b} + \Delta\mathbf{b}$
- How much is the output $\mathbf{x}$ perturbed?

Condition number of linear systems II

- We have

$$\mathsf{A}(\mathbf{x} + \Delta\mathbf{x}) = \mathbf{b} + \Delta\mathbf{b}$$

- Since $\mathsf{A}\mathbf{x} = \mathbf{b}$, we find

$$\mathsf{A}(\Delta\mathbf{x}) = \Delta\mathbf{b}$$

- Hence

$$\Delta\mathbf{x} = \mathsf{A}^{-1}(\Delta\mathbf{b})$$

Condition number III

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$$\kappa = \frac{\|\Delta \mathbf{x}\| / \|\mathbf{x}\|}{\|\Delta \mathbf{b}\| / \|\mathbf{b}\|}$$

- Using $\mathbf{b} = \mathsf{A}\mathbf{x}$ we get

$$\kappa = \frac{\|\mathsf{A}^{-1}\Delta \mathbf{b}\| \|\mathsf{A}\mathbf{x}\|}{\|\mathbf{x}\| \|\Delta \mathbf{b}\|}$$

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- Define the **condition number of matrix** A:

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

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Residual

- Suppose we are solving $A\mathbf{x} = \mathbf{b}$
- Suppose have approximate solution $\hat{\mathbf{x}}$
- As usual, do not know how far $\mathbf{x}$ is from true solution
- i.e. **forward error** $\hat{\mathbf{x}} - \mathbf{x}$
- Instead, only know the **residual**

$$\mathbf{r} := A\hat{\mathbf{x}} - \mathbf{b}$$

Backward error

- We see that $\hat{\mathbf{x}}$ **exactly** solves a **perturbed problem**:

$$A\hat{\mathbf{x}} = \mathbf{b} - \mathbf{r}$$

- Relative error is

$$\frac{\|\Delta \mathbf{x}\|}{\|\mathbf{x}\|} = \frac{\|\hat{\mathbf{x}} - \mathbf{x}\|}{\|\mathbf{x}\|} \leq \kappa(A)\frac{\|\mathbf{r}\|}{\|\mathbf{b}\|}$$

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- So forward error can be large even when backward error is small, if $\kappa(A)$ is large

Stability of algorithms

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  - a sequence of steps = mini-problems

- Conditioning of a problem is *independent* of any algorithm for solving that problem

- An algorithm replaces ϕ with an alternative problem $\widehat{\phi}$
- The result cannot be better than given by the condition number
- If an algorithm is much **worse** than expected from conditioning, the algorithm is **unstable**; otherwise it's

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- $x_\_$ is not affected by catastrophic cancellation (sum of two quantities of a similar size)
- Can we calculate x_+ from $x_\_$?
- Factor the quadratic as $f(x) = a(x - x_\_)(x - x_+)$
- Then $a\, x_\_\, x_+ = c$, so $x_+ = \frac{c}{a\, x_\_}$

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- So far we have studied the **forward error** $\Delta y := \hat{y} - y$
- Instead, we can take an alternative viewpoint:
  - "calculated result = exact solution for nearby input?"
- i.e. want **backward error** Δx such that

$$\hat{y} = f(x + \Delta x)$$

Summary

- Condition number for a problem: Sensitivity of output to input
- Catastrophic cancellation in subtraction and its avoidance
- Condition number for summation, quadratics and linear solve

- Stability
- Backward error