9. Conditioning and stability

9. Conditioning and stability

Last time

- Rules for derivatives via new algebra
- Dual numbers
- Implementation
- Directional derivatives, partial derivatives, jacobians

Goals for today

Conditioning: Sensitivity of problems

Catastrophic cancellation

■ Suppose have (numerical) problem given by function ϕ :

- Suppose have (numerical) problem given by function ϕ :
- Given input x, calculate output $y = \phi(x)$

- Suppose have (numerical) problem given by function ϕ :
- $\blacksquare \ \ \text{Given input } x \text{, calculate output } y = \phi(x)$
- How sensitive is output to input?

- lacksquare Suppose have (numerical) problem given by function ϕ :
- $\blacksquare \ \ \text{Given input } x \text{, calculate output } y = \phi(x)$
- How **sensitive** is output to input?

- Suppose perturb input by Δx .
- How large is resulting effect Δy on output?

- Suppose have (numerical) problem given by function ϕ :
- $\blacksquare \ \ \text{Given input } x \text{, calculate output } y = \phi(x)$
- How sensitive is output to input?

- Suppose perturb input by Δx .
- How large is resulting effect Δy on output?

Example: Intersection of two thick lines at angle

Absolute errors

- \blacksquare Suppose \hat{x} is approximation of input x
- lacksquare Define $\Delta x := \hat{x} x$ as error on the input

Absolute errors

- \blacksquare Suppose \hat{x} is approximation of input x
- lacksquare Define $\Delta x := \hat{x} x$ as error on the input

 \blacksquare Calculated output is $\hat{y} := \phi(\hat{x}) = \phi(x + \Delta x)$

Absolute errors

- \blacksquare Suppose \hat{x} is approximation of input x
- \blacksquare Define $\Delta x := \hat{x} x$ as error on the input
- \blacksquare Calculated output is $\hat{y} := \phi(\hat{x}) = \phi(x + \Delta x)$

lacksquare Δx and Δy are absolute errors

lacksquare Size of absolute error Δy depends on size of input

- Size of absolute error Δy depends on size of input
- Usually more interested in relative errors

- Size of absolute error Δy depends on size of input
- Usually more interested in relative errors
- Divide absolute error by true value:

$$\delta x := \frac{\Delta x}{x} = \frac{\hat{x} - x}{x}; \quad \delta y := \frac{\Delta y}{y} = \frac{\hat{y} - y}{y}$$

- Size of absolute error Δy depends on size of input
- Usually more interested in relative errors
- Divide absolute error by true value:

$$\delta x := \frac{\Delta x}{x} = \frac{\hat{x} - x}{x}; \quad \delta y := \frac{\Delta y}{y} = \frac{\hat{y} - y}{y}$$

 $\bullet \text{ So } \hat{x} = x + \Delta x = x(1 + \delta x)$

Significant / accurate digits

- \blacksquare Suppose have approximation \hat{x} of true value x
- How **accurate** is it? Relative error is $|\delta x| = |\frac{\hat{x} x}{x}|$

Significant / accurate digits

- lacksquare Suppose have approximation \hat{x} of true value x
- How **accurate** is it? Relative error is $|\delta x| = |\frac{\hat{x} x}{x}|$
- Express number of significant or accurate digits:

$$d = -\log_{10} \left| \frac{\hat{x} - x}{x} \right|$$

lacksquare Gives number of digits after which \hat{x} and x differ

Conditioning

- For some problems, perturbing input does not affect output too much: well-conditioned
- For others, perturbing input can change output drastically: ill-conditioned

Conditioning

- For some problems, perturbing input does not affect output too much: well-conditioned
- For others, perturbing input can change output drastically: ill-conditioned

How can we measure conditioning?

- lacktriangle Given problem ϕ at input x
- Define absolute condition number $\hat{\kappa}_{\phi}(x)$:

- lacksquare Given problem ϕ at input x
- Define absolute condition number $\hat{\kappa}_{\phi}(x)$:

$$\hat{\kappa}_{\phi}(x) = \frac{\|\Delta y\|}{\|\Delta x\|}$$

- lacktriangle Given problem ϕ at input x
- Define absolute condition number $\hat{\kappa}_{\phi}(x)$:

$$\hat{\kappa}_{\phi}(x) = \frac{\|\Delta y\|}{\|\Delta x\|}$$

- $\|\cdot\|$ are suitable **norms** measuring length of vectors
- For real numbers, just take absolute value

- lacksquare Given problem ϕ at input x
- Define absolute condition number $\hat{\kappa}_{\phi}(x)$:

$$\hat{\kappa}_{\phi}(x) = \frac{\|\Delta y\|}{\|\Delta x\|}$$

- $\blacksquare \parallel \cdot \parallel$ are suitable **norms** measuring length of vectors
- For real numbers, just take absolute value

 $\blacksquare \ \hat{\kappa}_{\phi}(x,\epsilon)$: take maximum over inputs $\|\Delta x\| < \epsilon$

■ What happens if input $|\Delta x| \to 0$?

- What happens if input $|\Delta x| \to 0$?
- $\blacksquare \text{ Have } \Delta y = \phi(x + \Delta x) \phi(x)$

- What happens if input $|\Delta x| \to 0$?
- $\blacksquare \text{ Have } \Delta y = \phi(x+\Delta x) \phi(x)$
- \blacksquare So $\Delta y = \phi'(x) \, \Delta x$ to first order

- What happens if input $|\Delta x| \to 0$?
- $\blacksquare \text{ Have } \Delta y = \phi(x + \Delta x) \phi(x)$
- lacksquare So $\Delta y = \phi'(x) \, \Delta x$ to first order

 $\blacksquare \text{ Hence } \hat{\kappa}_{\phi}(x) = |\phi'(x)|$

Relative condition number

lacktriangle Define **relative condition number** $\kappa_\phi(x)$ by

$$\kappa_{\phi}(x) = \frac{\|\delta y\|}{\|\delta x\|}$$

■ Here we have the *relative* errors on top and bottom

Relative condition number

lacktriangle Define **relative condition number** $\kappa_\phi(x)$ by

$$\kappa_\phi(x) = \frac{\|\delta y\|}{\|\delta x\|}$$

Here we have the relative errors on top and bottom

■ Taking limit as $|\Delta x| \to 0$, obtain

$$\kappa_{\phi}(x) = \lim_{\Delta x \to 0} \left| \frac{\frac{\phi(x + \Delta x) - \phi(x)}{\phi(x)}}{\frac{\Delta x}{x}} \right| = \left| \frac{x \, \phi'(x)}{\phi(x)} \right|$$

Relative condition number

lacktriangle Define **relative condition number** $\kappa_\phi(x)$ by

$$\kappa_\phi(x) = \frac{\|\delta y\|}{\|\delta x\|}$$

Here we have the relative errors on top and bottom

■ Taking limit as $|\Delta x| \to 0$, obtain

$$\kappa_{\phi}(x) = \lim_{\Delta x \to 0} \left| \frac{\frac{\phi(x + \Delta x) - \phi(x)}{\phi(x)}}{\frac{\Delta x}{x}} \right| = \left| \frac{x \, \phi'(x)}{\phi(x)} \right|$$

Example: Condition number of addition

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

Example: Condition number of addition

- Addition of two numbers is a very basic operation
- We hope that it is well-conditioned. Is it?
- lacksquare Take problem $\phi(x)=x+a$ with a fixed a
- $\blacksquare = a + (x + \Delta x) (a + x) = \Delta x$
- lacktriangle Abs. condition number $\hat{\kappa}_{\phi} = |\phi'(x)| = 1$ well-behaved
- But we really care about relative condition number

Condition number of addition II

- Problem $\phi(x) = a + x$ with fixed a
- But relative condition number is

$$\kappa_{\phi} = \left| \frac{x \, \phi'(x)}{\phi(x)} \right| = \left| \frac{x}{a+x} \right|$$

- Note: $\phi(x)$ appears in *denominator*
- So κ is *large* when $x \simeq -a$
- Catastrophic cancellation: loss of digits of accuracy when subtracting two numbers that are close together
- Common task in numerical analysis: identify + eliminate catastrophic cancellation

Revisiting quadratic equations

Let's revisit the topic of solving quadratic equations

$$f(x) = ax^2 + bx + c = 0$$

 \blacksquare Problem ϕ : inputs: (a,b,c); outputs: roots x_\pm

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

Revisiting quadratic equations

Let's revisit the topic of solving quadratic equations

$$f(x) = ax^2 + bx + c = 0$$

 \blacksquare Problem ϕ : inputs: (a,b,c); outputs: roots x_\pm

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

What can go wrong?

Revisiting quadratic equations

Let's revisit the topic of solving quadratic equations

$$f(x) = ax^2 + bx + c = 0$$

 \blacksquare Problem ϕ : inputs: (a,b,c); outputs: roots x_\pm

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

- What can go wrong?
- \blacksquare Intuitively: if b>0 and ac is small, then x_+ suffers from catastrophic cancellation

Revisiting quadratic equations

Let's revisit the topic of solving quadratic equations

$$f(x) = ax^2 + bx + c = 0$$

 \blacksquare Problem ϕ : inputs: (a,b,c); outputs: roots x_\pm

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

What can go wrong?

 \blacksquare Intuitively: if b>0 and ac is small, then x_+ suffers from catastrophic cancellation

Eliminating cancellation for quadratics

- The root x_{-} is unaffected by catastrophic cancellation (sum of two quantities of similar size)
- \blacksquare Can we calculate x_+ from x_- ?

Eliminating cancellation for quadratics

- The root x_{-} is unaffected by catastrophic cancellation (sum of two quantities of similar size)
- \blacksquare Can we calculate x_+ from x_- ?
- \blacksquare Factor quadratic as $f(x) = a(x-x_-)(x-x_+)$
- $\blacksquare \text{ Then } a\,x_-\,x_+ = c \text{, so } x_+ = \frac{c}{a\,x_-}$

Condition number of quadratic equations

How calculate condition number of root of quadratic equation?

Condition number of quadratic equations

- How calculate condition number of root of quadratic equation?
- Suppose move a to $a + \Delta a$
- Root x_+ moves to $x_+ + \Delta x_+$

Condition number of quadratic equations

- How calculate condition number of root of quadratic equation?
- lacksquare Suppose move a to $a+\Delta a$
- $\blacksquare \ \, \text{Root} \, x_+ \, \text{moves to} \, x_+ + \Delta x_+ \,$
- $\blacksquare \kappa = \left| \frac{x_+}{a} \frac{\partial x_+}{\partial a} \right|$
- \blacksquare Find $\kappa = \left|\frac{x_+}{x_+ x_-}\right|$
- So condition number is large when roots are close
- Visualize by perturbing function near double root

Stability of algorithms

- Notion of "condition number" refers to a problem
- Solving a problem on the computer needs an algorithm
- Conditioning is independent of the algorithm

Stability of algorithms

- Notion of "condition number" refers to a problem
- Solving a problem on the computer needs an algorithm
- Conditioning is independent of the algorithm
- \blacksquare An algorithm replaces problem ϕ with alternative $\hat{\phi}$
- In general the result cannot be better than the condition number suggests
- If algorithm is much worse than expected from conditioning, algorithm is unstable; otherwise stable

Backward error

- A very useful point of view is that of backward error:
- \blacksquare Suppose algorithm $\hat{\phi}$ approximates a problem ϕ
- \blacksquare Then $\hat{y}:=\hat{\phi}(x)$ approximates exact result $y:=\phi(x)$

Backward error

- A very useful point of view is that of backward error:
- \blacksquare Suppose algorithm $\hat{\phi}$ approximates a problem ϕ
- \blacksquare Then $\hat{y}:=\hat{\phi}(x)$ approximates exact result $y:=\phi(x)$
- lacksquare So far have studied forward error $\Delta y := \hat{y} y$

Backward error

- A very useful point of view is that of backward error:
- \blacksquare Suppose algorithm $\hat{\phi}$ approximates a problem ϕ
- \blacksquare Then $\hat{y}:=\hat{\phi}(x)$ approximates exact result $y:=\phi(x)$
- lacksquare So far have studied forward error $\Delta y := \hat{y} y$
- Instead: "calculated result = exact solution for nearby input?"
- lacktriangle i.e. want **backward error** Δx such that

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

Summary

- (Absolute and relative) condition number for a problem
- Catastrophic cancellation in subtraction and its avoidance
- Stability
- Backward error