

IE5268 Theory and Algorithms for Nonlinear Optimization

Week 1: Course Overview & Introduction

Instructor: Guanyi Wang[†]

Department of Industrial Systems Engineering and Management (ISEM) † , National University of Singapore (NUS), Singapore.

Teaching Staff & Teaching Assistants

Teaching Instructor:

■ Instructor: Dr Guanyi Wang

■ Email: guanyi.w@nus.edu.sg

Office: E1-07-16

Office-Hour: Monday after the lecture

Teaching Assistant:

Mr Renyuan Li

■ Email: renyuan.li@u.nus.edu

Office-Hour: TBD

(Will be updated on Canvas)

Canvas & Assessments

NUS Canvas website:

Course code: IE 5268

Announcements

■ Files (Will be uploaded to Canvas)

Recording (Will be uploaded to Canvas)

Assessments:

Assignments: 40% (2 assignments, 20% each)

■ Midterm Take-home Quiz: 30%

30% (Week 7)

■ Final Take-home Quiz: 30%

(Week 13)

Textbooks

Required:

- Nocedal, Jorge, and Stephen J. Wright, eds. Numerical optimization. New York, NY: Springer New York, 1999.
- Y. Nesterov, Introductory Lectures on Convex Optimization: A Basic Course, Kluwer Academic Publishers, Norwell, MA, (2004)

Supplementary/Optional:

- A. Ruszcynski, Nonlinear Optimization, Princeton University Press, Princeton, NJ (2006)
- D. P. Bertsekas, Nonlinear Programming, Second Edition, Athena Scientific, Belmont, MA, (1999)

Module Outline

- Week 1: Overview & Introduction
- Week 2 6: Unconstrained Optimization
 - Week 2: Convex Analysis I & Optimality Conditions
 - Week 3: Gradient Method
 - Week 4: Proximal Gradient Method
 - Week 5: Stochastic Gradient Method
 - Week 6: Newton's Method
- Week 7: Review for first-half & Take home midterm (2 days)
- Week 8 12: Convex Constrained Optimization
 - Week 8: Convex Analysis II
 - Week 9: Constrained Convex Optimization
 - Week 10: Duality
 - Week 11: Equality Constrained Minimization
 - Week 12: Decomposition method
- Week 13: Review for second-half & Take home final (2 days)

Course Learning Outcomes

What I expect you to achieve after taking this course ...

- (Basic Results) Have a comprehensive knowledge to the basic results for different optimization methods
- (Optimality Conditions) Understand the necessary and sufficient optimality conditions for unconstrained and constrained optimization problems
- (Duality) Understand the duality theory for optimization problems
- (Large-scale Opt) Familiar with methods for large-scale optimization problems
- (Make Your Choice) Able to pick appropriate optimization methods based on given conditions/settings

Pre-requirements: Topics that I expect you have already known

Will be frequently used in this course. If you are not familiar with the following knowledge, this course will take you additional effort ...

Pre-requirements

MA3210 Mathematical Analysis II

- derivatives, gradients, Jacobians, Hessians
- Taylor's expansion
- sequences (subsequences, boundedness, accumulation points, etc.)
- continuity and limits

MA4230 Matrix Computation (Linear Algebra)

- vectors and vector norms, matrices and matrix norms
- matrix properties, e.g., symmetric, positive (semi) definite, (non)singular, etc.
- determinants, eigenvalues, and eigenvectors
- matrix factorizations
- condition number of a matrix

■ IE4210 Operations Research II

(Recommended)

- convex and concave function
- format of linear/nonlinear programming

Introduction to Nonlinear Unconstrained Optimization

Brief Introduction – 1

Basic Problem:

$$\min_{x \in \mathbb{R}^n} f(x)$$

- decision variable $x \in \mathbb{R}^n$
- objective function $f: \mathbb{R}^n \to \mathbb{R}$
- maximizing can be transferred into minimization, i.e., $\max_x \widehat{f}(x) = \min_x -\widehat{f}(x)$
- **Definition (global minimizer):** The vector x^* is a global minimizer if $f(x^*) \le f(x)$ such that $x \in \mathbb{R}^n$.
- **Definition (local minimizer):** For some given $\epsilon > 0$, the vector x^* is a local minimizer if $f(x^*) \le f(x)$ for all $x \in ||x x^*|| \le \epsilon$.
- **Definition (strict local minimizer):** For some given $\epsilon > 0$, the vector x^* is a strict local minimizer if $f(x^*) < f(x)$ for all $x \neq x^*$ such that $x \in ||x x^*|| \le \epsilon$.

Brief Introduction – 2

Recall the basic problem:

$$\min_{x \in \mathbb{R}^n} f(x)$$

- Notation (without specific comments, not always hold in this course or references)
 - Gradient: $g(x) := \nabla f(x) \in \mathbb{R}^n$ ■ Hessian: $H(x) := \nabla^2 f(x) \in \mathbb{R}^{n \times n}$
- **Assumptions:** we will always assume that f is a continuous function
- Going to see the following three types of *f*:
 - *f* is once or twice continuously differentiable (smooth optimization)
 - f is non-differentiable but with structure (structured non-smooth optimization)
 - derivatives of f are too expensive or unavailable (derivative free optimization)

Examples for above three types of objective f

Data Fitting Example - Asteroid Ceres

In January 1801: Asteroid Ceres is discovered, but in Autumn 1801 it "disappeared". Gauss considers an elliptic orbit instead of a circular orbit

circular orbit:
$$x^2 + y^2 = r$$
 for some $r > 0$ elliptic orbit: $\alpha x^2 + \beta y^2 + \gamma xy = 1$ for some α, β, γ

How did Gauss do it?

- used a collection of N previous location measurements $(x_1, y_1), (x_2, y_2), \dots, (x_N, y_N)$.
- find the "best" α, β, γ that satisfy

$$(\alpha^*, \beta^*, \gamma^*) := \operatorname*{arg\,min}_{\alpha, \beta, \gamma} \frac{1}{N} \sum_{i=1}^{N} \left(\alpha x_i^2 + \beta y_i^2 + \gamma x_i y_i - 1 \right)^2,$$

which is nonlinear and twice continuously differentiable

■ looked for Ceres along the ellipse defined by $\alpha^*x^2 + \beta^*y^2 + \gamma^*xy = 1$

Speech recognition: Multi-Class Regression – 1

Consider the following problem ...

- Number of classes $N_c \approx 100$ (basic units of sound)
- Number of features $N_f \approx 10^4$ (coefficients in the mathematical representation of a digital sample of sound)
- Number of parameters $N_p \approx 10^6$ (#classes × #features)
- Number of data points $N_d \approx 10^10$ and growing (size of data)
- Compute *w** as solution to

$$\max_{w \in \mathbb{R}^{N_p}} f(w) + \lambda \|w\|_1 \quad \lambda > 0$$
 is a sparsity parameter

where

$$f(w) := \sum_{i=1}^{N_d} \log \left(\frac{\exp(w_{y_i}^\top x_i)}{\sum_{j=1}^{N_c} \exp(w_j^\top x_i)} \right)$$

Speech recognition: Multi-Class Regression – 2

■ Predicted probability of new input \hat{x} being in class $k \in [N_c]$ is

$$\mathbb{P}(y = k \mid x = \widehat{x}) = \frac{\exp((w^*)_{y_i}^{\top} \widehat{x})}{\sum_{j=1}^{N_c} \exp((w^*)_j^{\top} \widehat{x})}$$

- Major challenges
 - $f(w) + \lambda ||w||_1$ is nonlinear
 - $||w||_1$ is non-smooth when $w_i = 0$ for some i (structured non-smooth)
 - Computing $\nabla f(w)$ is very expensive! Must sum up 10 billion gradients.

Tuning of algorithmic parameters

This is widely considered in machine learning ...

- Almost all numerical codes use various parameters
- The programmer must choose default values for these parameters
- The values chosen for the parameters are often crucial for excellent performance
- Sensible values for the parameters may be obtained by (approximately) solving

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\min_{x \in \mathbb{R}^n} f(x) := \mathsf{CPU-time}(x; \mathsf{solver}) \text{ or } \mathsf{ITER}(x; \mathsf{solver})
```

- n represents the number of parameters
- *p* represents the vector of problem parameters
- CPU-time represents the time required to solve a collection of test problems for a given value of the parameter vector *p*
- ITER represents the number of iterates required to solve a collection of test problems for a given value of the parameter vector *p*
- Computing the gradient of f is difficult (it is likely noisy and possibly non-differentiable)

Quick Summary of Nonlinear Unconstrained Optimization

Summary – 1

Unconstrained optimization problems may

- have a linear or nonlinear objective function
- be convex or nonconvex
- have an objective function that is twice continuously differentiable, once continuously differentiable, structurally non-smooth, non-smooth
- contain continuous and/or discrete variables
- vary in size
 - small size $\approx 1 \sim 10^2$ variables
 - median size $\approx 10^2 \sim 10^3$ variables
 - \blacksquare large size $\approx 10^3 \sim 10^6$ variables
 - lacktriangle very large size $\geq 10^6$ variables

Summary – 2

We may be interested in

- a local solution or global solution
- the minimum value of the objective function and/or the minimizer
- finding multiple distinct minimizers
- the lowest value of the objective given time constraints or limits on the number of allowed evaluations of the objective function

Background and Basics for Optimization: Computer Arithmetic

Modern computers store real numbers as

$$x = \pm \left(d_0 + \frac{d_1}{\beta_1} + \dots + \frac{d_{p-1}}{\beta_{p-1}}\right) \beta^E.$$

- base: β (e.g., 2)
- significand precision: p (e.g., 24 (SP), 53 (DP))
- exponent: $E \in [L, U]$ (e.g., [-126, 127] (SP), [-1022, 1023] (DP))
- $d_i \in \{0, ..., \beta 1\}$ for i = 0, ..., p 1
- lacktriangleright the floating-point system is completely characterized by the four integers eta, $m{p}$, L, U
- lacksquare mantissa $d_0d_1\cdots d_{p-1}$
- fraction $d_1 \cdots d_{p-1}$
- floating-point system is normalized if d_0 is always nonzero unless the number represented is zero
- we will only consider normalized floating-point systems

Consider the following example with

$$\beta = 10$$
, $p = 4$, $L = -99$, $U = 99$

Some numbers

$$1 = 1.000 \times 10^{00}$$
$$34.67 = 3.467 \times 10^{01}$$
$$0.0346 = 3.460 \times 10^{-02}$$

smallest positive number

$$1.000 \times 10^{-99}$$

largest positive number

$$9.999 \times 10^{99}$$

Facts about floating-point systems

- It is finite, i.e, not all real numbers can be stored
- Machine numbers are those real numbers that may be exactly represented
- \blacksquare Floating-point numbers are equally spaced only between successive powers of β
- Total number of normalized floating-point numbers is

$$2(\beta-1)\beta^{p-1}(U-L+1)+1$$

- Smallest positive number: UFL = β^L underflow level
 - numbers smaller than UFL stored as zero
 - often not serious, because zero is a good approximation
- Largest number: $OFL = \beta^U (1 \beta^{-p})$ overflow level
 - numbers larger than OFL may not be stored
 - serious problem, compilers typically terminate

Rounding

When a real number x is not exactly representable, it is approximated by a "nearby" floating-point number fl(x). This process is called rounding and the error that is introduced is called rounding error.

- Common rounding strategies:
 - chopping: fl(x) is obtained by truncating the expansion of x after d_{p-1} . Also called round-to-zero. Widely-used in neural network training.
 - round-to-nearest: fl(x) is the closest floating-point number to x. In case of a tie, use the floating-point number whose last stored digit is even. Also called round-to-even
- Assume round-to-nearest in our course since it is the most accurate and the default rounding rule on machines

Question: How bad can the rounding error be? **Answer:** Involves the concept of machine precision.

Machine precision assuming round-to-nearest

The machine precision is defined as $\epsilon:=\frac{1}{2}\beta^{1-p}$, which bounds the relative error in storing a floating-point number

$$\frac{|\mathsf{fl}(x) - x|}{|x|} \le \epsilon.$$

The machine precision ϵ is equal to

- lacktriangle the liminf such that $\mathrm{fl}(1+\epsilon)>1$
- lacksquare the the largest number such that $\mathrm{fl}(1+\epsilon)=1$
- half the distance between 1 and the nearest floating-point number

For example, using round-to-nearest, p=4 and $\beta=10$, we have

$$1.000 + 0.0005 = 1.0005 \stackrel{\text{comp}}{=} 1$$

 $1.000 + 0.00051 = 1.00051 \stackrel{\text{comp}}{=} 1.001$

with
$$\epsilon = \frac{1}{2} \times 10^{1-4} = 0.0005$$
.

Exceptional values in the floating-point system

Institute of Electrical and Electronics Engineers (IEEE) standard allows for the following exceptional values:

- Inf: represents "infinity" and results from dividing a finite number by zero
- NaN: stands for "not a number" and results from undefined or not well-defined operations, e.g., 0/0, $0 \times \infty$, ∞/∞ .

Floating-point addition & multiplication: Let $x=4.452\times 10^{02}$ and $y=6.436\times 10^{-01}$

- Addition of two floating-point numbers (similar for subtraction)
 - shift so that exponents are the same, add, then re-normalize
 - for example

$$x + y = (4.452 \times 10^{02}) + (6.436 \times 10^{-01})$$
$$= (4.452 \times 10^{02}) + (0.006436 \times 10^{02})$$
$$= 4.458436 \times 10^{02} \stackrel{\text{comp}}{=} 4.458 \times 10^{02}$$

- generally, trailing digits of smaller (in magnitude) number are lost
- Multiplication of two floating-point numbers (similar for division)
 - exponents are summed and mantissas multiplied
 - product of two p digit mantissas is generally 2p digits (must round)
 - for example

$$x \times y = (4.452 \times 10^{02}) \times (6.436 \times 10^{-01})$$

= $28.653072 \times 10^{01} = 2.8653072 \times 10^{02} \stackrel{\text{comp}}{=} 2.865 \times 10^{02}$

Background and Basics for Optimization: Linear systems, norms, and condition numbers

The problem of interest: Given a data matrix $A \in \mathbb{R}^{n \times n}$ and $b \in \mathbb{R}^n$, solve the linear system Ax = b.

- We use a_{ij} to denote the component of A in row i and column j
- Can consider questions of existence and uniqueness of solutions
- What about conditioning (sensitivity of the solution)
- If A is nonsingular, A^{-1} exists and the unique solution is $x = A^{-1}b$ Consider the following example:

$$\begin{cases} x_1 + 3x_2 = 5 \\ 2x_1 + 7x_2 = 3 \end{cases} \Rightarrow Ax = b$$

where

$$n=2, \quad A=\begin{pmatrix} 1 & 3 \\ 2 & 7 \end{pmatrix}, \quad x=\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, \quad b=\begin{pmatrix} 5 \\ 3 \end{pmatrix}$$

Is the solution unique?

Nonsingular case

A square matrix $A \in \mathbb{R}^{n \times n}$ is said to be nonsingular if any of the following equivalent conditions are satisfied:

- The inverse matrix A^{-1} exists
- \bullet det(A) \neq 0
- ightharpoonup rank(A) = n
- $Az = 0 \Rightarrow z = 0$
- $z \neq 0 \Rightarrow Az \neq 0$

If A is nonsingular, then Ax = b has a unique solution.

Singular case

A square matrix $A \in \mathbb{R}^{n \times n}$ is said to be singular, then

- if $b \in \text{span}(A)$, then infinitely many solutions exist
- if $b \notin \text{span}(A)$, then no solutions exist

Consider the following example:

$$\underbrace{\begin{pmatrix} 1 & 3 \\ 2 & 6 \end{pmatrix}}_{A} \underbrace{\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}}_{x} = \underbrace{\begin{pmatrix} b_1 \\ b_2 \end{pmatrix}}_{b}$$

- lacktriangledown det $(A) = 0 \Rightarrow A$ is singular
- If $b = \begin{pmatrix} 4 \\ 8 \end{pmatrix}$ \Rightarrow $x = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$, $x = \begin{pmatrix} 4 \\ 0 \end{pmatrix}$, or ... infinitely many solutions.
- If $b = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$, then no solutions.

"Known" material for square A

- general A: solve Ax = b using A = LU factorization by Gaussian elimination method
- positive-definite A: solve Ax = b using $A = LL^{\top}$ by Cholesky factorization

New material for square A

- Conditioning: when is the solution x to the system Ax = b sensitive to the input data A and b?
- To understand conditioning, we will introduce the condition number of a matrix A

$$cond(A) := ||A|| ||A^{-1}||$$

- This requires us to understand matrix norms ||A||
- Which requires us to understand vector norms

Examples of vector norm

In linear algebra, we know many vector norms

$$||x||_2 = \sqrt{x_1^2 + x_2^2 + \dots + x_n^2}$$

 ℓ_2 -norm

$$||x||_1 = |x_1| + |x_2| + \cdots + |x_n|$$

 ℓ_1 -norm

$$||x||_{\infty} = \max_{i=1}^{n} |x_i|$$

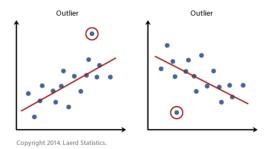
 ℓ_∞ -norm

For example, let

$$x = \begin{pmatrix} -12 \\ -3 \\ 4 \end{pmatrix}, \quad ||x||_2 = 13, \quad ||x||_1 = 19, \quad ||x||_{\infty} = 12$$

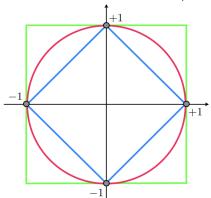
Sometimes a specific norm may be better than another ...

Suppose we have accumulated data as the result of a carefully designed experiment, and then obtained a model of the data.



If we store the error of each data point (of right-hand-side figure) in the vector $x=(10^{-2},10^{-1},\ldots,\mathbf{1},\ldots,10^{-1})$. We get $\|x\|_{\infty}=\mathbf{1}$ by outlier. Maybe better to consider $\|x\|_2/n$?

Geometry of different types of ℓ_p -norms



Some results:

- $||x||_{\infty} \le ||x||_2 \le ||x||_1$
- $||x||_1 \le \sqrt{n}||x||_2$
- $||x||_2 \le \sqrt{n} ||x||_{\infty}$
- $||x||_1 \le n||x||_{\infty}$

5/44

Vector norm

A vector norm is any real-valued function $\|\cdot\|$ of a vector that satisfies the following properties:

- if $x \neq 0$, then ||x|| > 0
- $\|x+y\| \le \|x\| + \|y\|$ (triangle inequality)
- Using the above properties, it may be shown that
 - $\|x\| = 0$ if and only if x = 0
 - $\qquad \|x\|-\|y\|\leq |\|x\|-\|y\||\leq \|x-y\| \qquad \text{(reverse triangle inequality)}$
- We have already seen some examples $\ell_1, \ell_2, \ell_\infty$ norms satisfy the definition of vector norm.

Induced matrix norm

Given a vector norm ||x||, we define the induced matrix norm of A as

$$||A|| := \max_{||x||=1} ||Ax||$$

- Measures the maximum amount of "elongation" resulting from multiplication by A
- It can be shown that
 - $\|A\|_1 = \max_{1 \le j \le n} \sum_{i=1}^n |a_{ij}| \text{ maximum absolute column sum}$
 - $\|A\|_{\infty}=\max_{1\leq i\leq n}\sum_{j=1}^{n}|a_{ij}|$ maximum absolute row sum

Consider the following example:

$$A = \begin{pmatrix} -7 & 4 & 3 & 1 \\ 8 & -5 & 6 & 0 \\ -1 & -3 & 7 & 4 \\ 5 & 0 & 0 & -5 \end{pmatrix} \quad \text{with} \quad ||A||_1 = 21, \quad ||A||_{\infty} = 19$$

Matrix norm

A matrix norm is any real-valued function $\|\cdot\|$ of a matrix that satisfies the following properties:

- if $A \neq 0$, then ||A|| > 0
- $\blacksquare \|A + B\| \le \|A\| + \|B\| \qquad \text{(triangle inequality)}$
- Using the above properties, it may be shown that
 - ||A|| = 0 if and only if A = 0
- We have already seen some examples $||A||_1$, $||A||_\infty$ norms satisfy the definition of vector norm.
- Induced matrix norms (not all norms) are consistent, i.e., satisfy
 - $||AB|| \le ||A|| ||B||$
 - $||Ax|| \le ||A|| ||x||$ for all x

Condition Number 1

Condition number

We define the condition number of a square matrix A as

$$\operatorname{cond}(A) := \left\{ \begin{array}{ll} \|A\| \|A^{-1}\| & \text{if } A \text{ is non-singular} \\ \infty & \text{if } A \text{ is singular} \end{array} \right.$$

- large condition number \Rightarrow A is nearly singular
- geometric interpretation: the condition number is the ratio of the largest stretching over the smallest shrinking caused by multiplication by A
- the residual $r := b A\hat{x}$ is not a reliable measure of accuracy
- for well-conditioned problems, the relative residual is reliable:

$$\frac{\|b - A\widehat{x}\|}{\|\widehat{x}\| \|A\|}$$

fact: backward stable algorithms produce small relative residuals

Condition Number 2

Properties of the condition number: If the condition number is defined by any induced matrix norm, then

- $oldsymbol{=}$ cond(I) = 1
- $lue{}$ cond(A) ≥ 1
- $cond(\alpha A) = cond(A)$ for all $\alpha \neq 0$
- If *D* is a diagonal matrix, then

$$\operatorname{cond}(D) = \frac{\max_{i=1}^{n} |d_{ii}|}{\min_{i=1}^{n} |d_{ii}|}$$

Consider the following example:

$$D = \begin{pmatrix} 2 & 0 & 0 \\ 0 & -40 & 0 \\ 0 & 0 & 0.01 \end{pmatrix} \quad \Rightarrow \quad \text{cond}(D) = \frac{|-40|}{|0.01|} = 4000$$

Condition Number 3

Computing the condition number

- Computing ||A|| is computationally cheap
- Computing A^{-1} is very computationally expensive
- It is more expensive to compute A^{-1} than it is to solve Ax = b
- Some software cheaply estimates cond(A) while solving Ax = b
 - LINPACK \rightarrow sgeco
 - $\blacksquare \ \mathsf{LAPACK} \to \mathsf{sgecon}$
 - $\blacksquare \ \mathsf{NAG} \to \mathsf{f07agf}$
 - $\blacksquare \mathsf{Matlab} \to \mathsf{condest}$
 - lacksquare Python ightarrow numpy.linalg.norm

Accuracy analysis 1

- Suppose we are given A,b and a perturbed right-hand-side $\hat{b}=b+\Delta b$
- Let x and \hat{x} satisfy

$$Ax = b \quad \Rightarrow \quad \|b\| = \|Ax\| \le \|A\| \|x\| \quad \text{(consistency)}$$
 $A\widehat{x} = \widehat{b}$

■ Define $\Delta x := \hat{x} - x$.

$$A\Delta x = A(\widehat{x} - x) = A\widehat{x} - Ax = \widehat{b} - b = \Delta b \quad \Rightarrow \quad \Delta x = A^{-1}\Delta b$$

 Using the previous equality, the consistency property, and consistency property,

$$\frac{\|\Delta x\|}{\|x\|} = \frac{\|A^{-1}\Delta b\|}{\|x\|} \le \frac{\|A^{-1}\|\|\Delta b\|}{\|x\|} \le \frac{\|A\|\|A^{-1}\|\|\Delta b\|}{\|b\|} \le \operatorname{cond}(A) \frac{\|\Delta b\|}{\|b\|}$$

Accuracy analysis 2

We proved the following perturbation result in the previous slide.

Theorem (Error bound for linear systems)

If A is nonsingular, Ax = b and $A\widehat{x} = \widehat{b}$, then

$$\frac{\|\Delta x\|}{\|x\|} \le \operatorname{cond}(A) \frac{\|\Delta b\|}{\|b\|}$$

A similar analysis shows the following.

Theorem (Error bound for linear systems)

If A is nonsingular, Ax = b and $A\hat{x} = \hat{b}$, then

$$\frac{\|\Delta x\|}{\|x\|} \le \operatorname{cond}(A) \frac{\|\widehat{A} - A\|}{\|A\|}$$

- Similar result holds when A and b are perturbed simultaneously
- What does this mean in terms of computer representation?

Accuracy analysis 3

What does this mean in terms of computer representation?

- We give the computer A and b and want to find x such that Ax = b. We assume that A is exactly representable, but that b is not.
- Define $\hat{b} := \mathsf{fl}(b)$ so that \hat{b} satisfies

$$\frac{\|\widehat{b} - b\|}{\|b\|} = \frac{\|\mathsf{fl}(b) - b\|}{\|b\|} \le \epsilon$$

- We solve $A\widehat{x} = \widehat{b}$
- From result on previous slide we know that

$$\frac{\|\Delta x\|}{\|x\|} \le \operatorname{cond}(A) \frac{\|\Delta b\|}{\|b\|} \le \operatorname{cond}(A)\epsilon$$