Matrix Computations

S. Bora

September-November 2020

This course will be concerned with the following standard problems:

Linear systems of equations

- Linear systems of equations
- Least squares problems

- Linear systems of equations
- Least squares problems
- Eigenvalue problems

- Linear systems of equations
- Least squares problems
- Eigenvalue problems
- Singular value problems

This course will be concerned with the following standard problems:

- Linear systems of equations
- Least squares problems
- Eigenvalue problems
- Singular value problems

The methods for solving these problems can be broadly classified as:

This course will be concerned with the following standard problems:

- Linear systems of equations
- Least squares problems
- Eigenvalue problems
- Singular value problems

The methods for solving these problems can be broadly classified as:

Direct methods

This course will be concerned with the following standard problems:

- Linear systems of equations
- Least squares problems
- Eigenvalue problems
- Singular value problems

The methods for solving these problems can be broadly classified as:

- Direct methods
- Iterative methods

The following general topics will recur all throughout.

Matrix factorizations

- Matrix factorizations
- Effects of finite precision arithmetic on the algorithms

- Matrix factorizations
- Effects of finite precision arithmetic on the algorithms
- Stability of the algorithms

- Matrix factorizations
- Effects of finite precision arithmetic on the algorithms
- Stability of the algorithms
- Perturbation theory and condition numbers

- Matrix factorizations
- Effects of finite precision arithmetic on the algorithms
- Stability of the algorithms
- Perturbation theory and condition numbers
- Speed of algorithms

Most of the methods for solving the problems aim to express *A* as a product of 'simpler' matrices which readily reveal the solution of the problem.

▶ LU decomposition (A = LU).

- ► LU decomposition (A = LU).
- QR decomposition (A = QR).

- ► LU decomposition (A = LU).
- ▶ QR decomposition (A = QR).
- ▶ The Schur decomposition ($A = UTU^*$).

- ▶ LU decomposition (A = LU).
- QR decomposition (A = QR).
- ▶ The Schur decomposition ($A = UTU^*$).
- ▶ The eigendecomposition $(A = XDX^{-1})$

- ▶ LU decomposition (A = LU).
- ▶ QR decomposition (A = QR).
- ▶ The Schur decomposition ($A = UTU^*$).
- ▶ The eigendecomposition $(A = XDX^{-1})$
- ▶ The Singular Value decomposition (SVD) ($A = USV^*$).

Rounding: The Silent Killer

Arithmetic operations on computers are inexact and messy. For example, computing

$$a+b$$

on a computer produces

$$(a+b)(1+e)$$

where *e* is called the rounding error.

Rounding: The Silent Killer

Arithmetic operations on computers are inexact and messy. For example, computing

$$a+b$$

on a computer produces

$$(a+b)(1+e)$$

where e is called the rounding error. The rounding error is bounded by $|\mathbf{e}| \leq \mathbf{u}$, where \mathbf{u} is the unit roundoff.

- ▶ Single precision: $\mathbf{u} \simeq \mathbf{5.96} \times \mathbf{10^{-8}}$
- ▶ Double precision: $\mathbf{u} \simeq 1.11 \times 10^{-16}$

Rounding: The Silent Killer

Arithmetic operations on computers are inexact and messy. For example, computing

$$a+b$$

on a computer produces

$$(a+b)(1+e)$$

where e is called the rounding error.

The rounding error is bounded by $|\mathbf{e}| \leq \mathbf{u}$, where \mathbf{u} is the unit roundoff.

- ▶ Single precision: $\mathbf{u} \simeq \mathbf{5.96} \times \mathbf{10^{-8}}$
- ▶ Double precision: $\mathbf{u} \simeq 1.11 \times 10^{-16}$

IEEE standard allows to track small errors made when two numbers are added, subtracted, multiplied or divided on a computer.

The rules of arithmetic are lost on computers! For example, generally

The rules of arithmetic are lost on computers! For example, generally

$$\mathbf{a} + (\mathbf{b} + \mathbf{c}) \neq (\mathbf{a} + \mathbf{b}) + \mathbf{c}$$

 $\mathbf{a} \times (\mathbf{b} + \mathbf{c}) \neq \mathbf{a} \times \mathbf{b} + \mathbf{a} \times \mathbf{c}$
 $\mathbf{a} \times (\mathbf{b} \times \mathbf{c}) \neq (\mathbf{a} \times \mathbf{b}) \times \mathbf{c}$

The rules of arithmetic are lost on computers! For example, generally

$$\mathbf{a} + (\mathbf{b} + \mathbf{c}) \neq (\mathbf{a} + \mathbf{b}) + \mathbf{c}$$

 $\mathbf{a} \times (\mathbf{b} + \mathbf{c}) \neq \mathbf{a} \times \mathbf{b} + \mathbf{a} \times \mathbf{c}$
 $\mathbf{a} \times (\mathbf{b} \times \mathbf{c}) \neq (\mathbf{a} \times \mathbf{b}) \times \mathbf{c}$

On my computer MATLAB produces:

$$\begin{array}{rcl} (\frac{4}{3}-1)*3-1 &=& -2.2204\times 10^{-16} \\ 5\times \frac{(1+\exp(-50))-1}{(1+\exp(-50))-1} &=& \mbox{NaN}. \\ & \frac{\log(\exp(750))}{100} &=& \mbox{Inf}. \end{array}$$

For day-to-day ordinary computations things are not that bad. But things can go wrong. Safeguards must be taken against unpleasant results.

For day-to-day ordinary computations things are not that bad. But things can go wrong. Safeguards must be taken against unpleasant results.

Prevention is better than cure!

Stability of algorithms

Analysing the errors caused by the algorithm itself requires knowing the effect of rounding errors during the execution of the algorithm. A desirable property of algorithms is *backward stability:*

If an algorithm alg(x) is used to compute f(x), then including the effect of rounding error, alg(x) is said to be backward stable if $alg(x) = f(x + \delta x)$ for small δx . Here δx is called the backward error.

Stability of algorithms

Analysing the errors caused by the algorithm itself requires knowing the effect of rounding errors during the execution of the algorithm. A desirable property of algorithms is *backward stability:*

If an algorithm alg(x) is used to compute f(x), then including the effect of rounding error, alg(x) is said to be backward stable if $alg(x) = f(x + \delta x)$ for small δx . Here δx is called the backward error.

Thus a backward stable algorithm provides the exact answer to a slightly perturbed problem.

The computed solution to a problem provided by an algorithm is seldom its exact solution. The difference may be largely attributed to:

The computed solution to a problem provided by an algorithm is seldom its exact solution. The difference may be largely attributed to:

Error in input data arising from prior calculations, measurement errors and rounding errors due to finite precision arithmetic.

The computed solution to a problem provided by an algorithm is seldom its exact solution. The difference may be largely attributed to:

- Error in input data arising from prior calculations, measurement errors and rounding errors due to finite precision arithmetic.
- Errors introduced by the algorithm when making approximations.

The computed solution to a problem provided by an algorithm is seldom its exact solution. The difference may be largely attributed to:

- Error in input data arising from prior calculations, measurement errors and rounding errors due to finite precision arithmetic.
- Errors introduced by the algorithm when making approximations.

This makes it necessary to understand the sensitivity of the solution to perturbations in the input data. The condition number of a problem is a measure of this sensitivity.

The computed solution to a problem provided by an algorithm is seldom its exact solution. The difference may be largely attributed to:

- Error in input data arising from prior calculations, measurement errors and rounding errors due to finite precision arithmetic.
- Errors introduced by the algorithm when making approximations.

This makes it necessary to understand the sensitivity of the solution to perturbations in the input data. The condition number of a problem is a measure of this sensitivity.

Thus if the algorithm is backward stable, then the *forward error* which is the difference between its exact and computed solutions is small if the solution is not too sensitive to perturbation.

Speed of algorithms

The speed of an algorithm is traditionally measured in terms of the number of *floating point operations* or *flops* it performs. The design of every algorithm will be accompanied by an estimate of its *flop count*.

Speed of algorithms

The speed of an algorithm is traditionally measured in terms of the number of *floating point operations* or *flops* it performs. The design of every algorithm will be accompanied by an estimate of its *flop count*.

However it may take significantly longer to move the data to the point at which it is operated upon than to actually perform the operations. Therefore, the speed also greatly depends upon the order and manner of implementation of the operations.

Speed of algorithms

The speed of an algorithm is traditionally measured in terms of the number of *floating point operations* or *flops* it performs. The design of every algorithm will be accompanied by an estimate of its *flop count*.

However it may take significantly longer to move the data to the point at which it is operated upon than to actually perform the operations. Therefore, the speed also greatly depends upon the order and manner of implementation of the operations.

If an algorithm is *iterative*, then it is necessary to know the number of iterations necessary to accept any approximate solution as an answer. This is decided by the quality of the convergence, whether *linear*, *quadratic or cubic*....

Class timings

- The class timings are slot A (9a.m.-9:55 a.m. of Monday-Wednesday) for theory and slot A1 (2-4 p.m. on Tuesday) for lab.
- Additionally (9 a.m.-9:55 a.m) of Saturdays with Monday/Tuesday/Wednesday timetables are also reserved for the course.
- There will be no live classes. Instead lecture videos and slides will be posted to the class group on MS Teams on a regular basis.
- ► There will be interaction sessions on MS teams every week on Wednesdays (9-9:55 a.m. for theory) and Tuesdays (2p.m.-4 p.m. for lab).
- The other class timings will be utilized for assessments/tests.
- ► In the first week, the interaction will be on Monday (9a.m.-9:55 a.m.) for theory.



Texts & References and Evaluation Policy

Textbook:

 Fundamentals of Matrix Computations by D. S. Watkins (2nd or 3rd edition)

Texts & References and Evaluation Policy

Textbook:

 Fundamentals of Matrix Computations by D. S. Watkins (2nd or 3rd edition)

Reference books:

- Applied Numerical Linear Algebra by J. W. Demmel.
- Numerical Linear Algebra by L. N. Trefethen and D. Bau.
- Numerical Computing with IEEE floating point arithmetic by M. Overton.

Texts & References and Evaluation Policy

Textbook:

 Fundamentals of Matrix Computations by D. S. Watkins (2nd or 3rd edition)

Reference books:

- Applied Numerical Linear Algebra by J. W. Demmel.
- Numerical Linear Algebra by L. N. Trefethen and D. Bau.
- Numerical Computing with IEEE floating point arithmetic by M. Overton.

A detailed evaluation policy has already been posted.