

Numerical Methods

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Lecture 5

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Organisational

- Assignment 0 – discussion of the solutions

| | To appear | Submission DL |
|----------------|---------------|---------------|
| • Assignment 1 | online | 15.11 |
| • Assignment 2 | 6.12 | 10.1 |

Solving linear algebraic equations

→ The linear systems problem:

$$Ax = b$$

$$A = \begin{bmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1n} \\ a_{21} & a_{22} & a_{23} & \dots & a_{2n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & a_{m3} & \dots & a_{mn} \end{bmatrix}$$

$$x = \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} \quad b = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

- Some methods for solving linear systems and their features:
- Gaussian Elimination (pivoting, scaling)
 - Matrix factorisation, LU decomposition
 - Back/Forward substitution

Linear algebra: recall

→ The linear systems problem:

$$\mathbf{Ax} = \mathbf{b}$$

Theorem 1: Given the matrix $\mathbf{A} \in \mathbf{R}^{n \times n}$ the following statements are equivalent

1. \mathbf{A} is nonsingular;
2. The columns of \mathbf{A} form an independent set of vectors;
3. The rows of \mathbf{A} form an independent set of vectors;
4. The linear system $\mathbf{Ax} = \mathbf{b}$ has a unique solution for all vectors $\mathbf{b} \in \mathbf{R}^n$;
5. The linear system $\mathbf{Ax} = \mathbf{0}$ has only the trivial solution $\mathbf{x} = \mathbf{0}$;
6. The determinant of \mathbf{A} is nonzero: $\det \mathbf{A} \neq 0$.

Gauss elimination method

- ➔ Write the linear system as a single augmented matrix: $\mathbf{A}' = [\mathbf{A} | \mathbf{b}]$
- ➔ Apply the solution algorithm to \mathbf{A}' – combination of ***elementary row operations***:
 1. multiply row with a nonzero scalar c
 2. interchange two rows
 3. multiply a row by a nonzero scalar c and add the result to another row
- ➔ If we can obtain a matrix \mathbf{A}_2 from \mathbf{A}_1 applying 1.-3. then \mathbf{A}_1 and \mathbf{A}_2 are told to be ***row equivalent***
- ➔ ***Backward substitution (back-solve)***: process of computing the unknowns from a system that is in upper-triangular form is called

Gauss elimination method

→ Write the linear system as a single augmented matrix: $\mathbf{A}' = [\mathbf{A} | \mathbf{b}]$

Theorem 2. Let \mathbf{A}' be augmented matrix corresponding to a linear system $\mathbf{A}\mathbf{x}=\mathbf{b}$ and suppose that \mathbf{A}' is row equivalent to $\mathbf{A}'' = [\mathbf{T} | \mathbf{c}]$. Then the two systems have the same solution sets.

→ Special classes of matrices:

$$U = \begin{bmatrix} 1 & 2 & 3 \\ 0 & 4 & 5 \\ 0 & 0 & 6 \end{bmatrix}$$

→ Upper triangular(U):

$$L = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 3 & 0 \\ 4 & 5 & 6 \end{bmatrix}$$

→ Lower triangular(L):

→ Goal: Reduce augmented matrix \mathbf{A}' to the new augmented matrix $\mathbf{A}'' = [\mathbf{U} | \mathbf{c}]$ where \mathbf{U} is *upper triangular matrix*.

Naive Gauss elimination method

- See example shown in class and R code example in `tmp/NumericalMethods/TestingCode/Lecture7/`

```
#naive gaussian elimination
for (i in (1:(n-1))) #last column skipped - no elements below the diagonal
{
  for (j in ((i+1):n)) #down i-th column
  {
    m=a[j,i]/a[i,i] #compute the multiplier
    for (k in ((i+1):n))
      a[j,k]=a[j,k]-m*a[i,k] #eliminate a[j][i] element
    b[j]=b[j]-m*b[i] #right hand side is modified appropriately
  }
}
#backward solution algorithm
x[n]=b[n]/a[n,n]
for (i in (n-1):1)
{
  sum=0
  for (j in (i+1):n)
    sum=sum+a[i,j]*x[j]
  x[i]=(b[i]-sum)/a[i,i]
}
```

- Note that the algorithm does not create 0 in the lower triangular half of A → that would be waste of computer time!

- Backward solution (*back-solve*):
$$x_i = \frac{1}{a_{ii}} \left(b_i - \sum_{j=i+1}^n a_{ij} x_j \right)$$

Gauss elimination method - problems

- ➔ Possible problem: In the process of the backward reconstruction of the solution: we divide with the element on the diagonal
- ➔ If this element is 0, the algorithm breaks down
- ➔ Elements on the diagonal: pivot elements
- ➔ Solution: interchange two rows to avoid a zero element on the diagonal → **PIVOTING**
 - partial pivoting: entries below the diagonal in the same column are examined
 - complete pivoting: searches on current and all subsequent columns (more stable, but expensive to implement)
 - scaling (scaled pivoting): scaling the rows before pivoting to avoid catastrophic cancellations

Gauss elimination method - pivoting

Partial pivoting:

1. Suppose we are about to work on the i -th column. We search the portion of the i -th column below the diagonal and find an element with the largest absolute value. Assume this happens in the p -th row.
2. Interchange rows i and p
3. Proceed with elimination

Exercise 1: Add partial pivoting to the provided code for Gaussian elimination.

→ Total number of operations(mul.+div.+~~sub.~~): $\frac{1}{3}n^3 + O(n^2)$

LU Decomposition

- Gaussian elimination → altering right hand side (**b**)
- Several systems with the same coefficient matrix can be solved only if *all* right hand side vectors are known initially
- Cost of finding the inverse matrix: $AX=I$, $X=A^{-1}$ in addition to solving a single Gauss elimination system: $n^3 + O(n^2)$
- Total number of operations(mul.+div.): $\frac{1}{3}n^3 + O(n^2)$
- If elimination already performed, #additional op.: $n^2 + O(n^2)$

LU Decomposition

→ LU decomposition algorithm:

1. Factor the matrix A into the product of a lower triangular and upper triangular matrix: $A = LU$
2. Solve two triangular systems (instead of a full linear system): $Ax = b \rightarrow Ux = y$, where $Ly = b$
3. First solve $Ly = b$ and then $Ux = y$ to get the solution.

Exercises

Exercise 1: Add partial pivoting to the provided code for Gaussian elimination.

Exercise 2: Add partial pivoting to your LU decomposition code.

Exercise 3: Check if the code you wrote works properly using predefined R routine: `library('Matrix');`
`expand(lu(a))`