Computational Astrophysics

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May 12, 2019

Outline

Linear Systems of Equations

Linear systems of equations (LSEs) are everywhere:

- Interpolation (e.g., for the computation of the spline coefficients).
- ODEs (implicit time integration).
- Solution methods for elliptic PDEs.
- Solution methods for non-linear equations by linearization and Newton iterations.

Example applications in astrophysics are:

- Stellar structure and evolution
- Poisson solvers
- radiation transport and radiation-matter coupling
- nuclear reaction networks

Linear Systems of Equations

A system of linear equations can be written in matrix form

$$A\mathbf{x} = \mathbf{b} \;, \tag{1}$$

where, A is a real $n \times n$ matrix with coefficients a_{ij}. $\mathbf{b}$ is a given real vector and $\mathbf{x}$ is the vector of n unknowns.

Linear Systems of Equations

If $\det A = |A| \neq 0$ and $\mathbf{b} \neq 0$, the LSE has a unique solution

$$\mathbf{x} = A^{-1}\mathbf{b} \ , \tag{2}$$

where A^{-1} is the inverse of A with $AA^{-1} = A^{-1}A = \mathbf{I}$.

If $\det A = 0$, the equations either have no solution or an infinite number of solutions.

Matrix Inversion

The inverse of a matrix A is given by

$$A^{-1} = \frac{1}{|A|} \underbrace{\mathrm{adj} A}_{\text{adjugate}} \ . \tag{3}$$

the adjugate of A is the transpose of A's cofactor matrix C:

$$\mathrm{adj} A = C^T \ . \tag{4}$$

So the problem becomes finding C and $\det A$.

Cramer's Rule

LSEs of the kind

$$A\mathbf{x} = \mathbf{b} \ , \tag{5}$$

provided A is invertible (i.e., has non-zero $\det A$). The solution is

$$x_i = \frac{\det A_i}{\det A} \ , \tag{6}$$

where A_i is the matrix formed from A by replacing its i-th column by the column vector $\mathbf{b}$.
Cramer's rule is more efficient than matrix inversion. The latter scales in complexity with $n!$ (where n is the number of rows/columns of A), while Cramer's rule has been shown to scale with n^3, so is more efficient for large matrixes and has comparable efficiency to direct methods such as Gauss Elimination.

Cramer's Rule. Example

Consider the system

$$\begin{pmatrix} 5 & 3 & 4 \\ 2 & 1 & 5 \\ 5 & 4 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 3 \\ 4 \\ 2 \end{pmatrix} . \tag{7}$$

The determinant of the matrix A is

$$\det A = -14. \tag{8}$$

Therefore we will use Cramer's Rule to solve.

Cramer's Rule. Example

The solution for variable x_1 is given by

$$x_1 = \frac{\det A_1}{\det A} \ , \tag{9}$$

where A_1 is the matrix formed from A by replacing its first column by the column vector $\mathbf{b}$, i.e.

$$A_1 = \begin{pmatrix} 3 & 3 & 4 \\ 4 & 1 & 5 \\ 2 & 4 & 1 \end{pmatrix} . \tag{10}$$

This matrix has $\det A_1 = 17$ and therefore

$$x_1 = -\frac{17}{14}. \tag{11}$$

Cramer's Rule. Example

The solution for variable x_2 is given by

$$x_2 = \frac{\det A_2}{\det A} \ , \tag{12}$$

where A_2 is

$$A_2 = \begin{pmatrix} 5 & 3 & 4 \\ 2 & 4 & 5 \\ 5 & 2 & 1 \end{pmatrix} . \tag{13}$$

This matrix has $\det A_2 = -25$ and therefore

$$x_2 = \frac{25}{14}. \tag{14}$$

Cramer's Rule. Example

The solution for variable x_3 is given by

$$x_3 = \frac{\det A_3}{\det A} \ , \tag{15}$$

where A_3 is

$$A_3 = \begin{pmatrix} 5 & 3 & 3 \\ 2 & 1 & 4 \\ 5 & 4 & 2 \end{pmatrix} . \tag{16}$$

This matrix has $\det A_3 = -13$ and therefore

$$x_3 = \frac{13}{14}. \tag{17}$$

Cramer's Rule. Example

The complete solution is

$$\mathbf{x} = \frac{1}{14}\begin{pmatrix} -17 \\ 25 \\ 13 \end{pmatrix} . \tag{18}$$

Direct LSE Solvers

Direct methods consist of a finite set of transformations of the original coefficient matrix that reduce the LSE to one that is easily solved.

Gauss Elimination

Consider the following system,

$$A\mathbf{x} = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ 0 & a_{22} & a_{23} \\ 0 & 0 & a_{33} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix} . \tag{19}$$

This LSE is solved trivially by simple back-substitution:

$$x_3 = \frac{b_3}{a_{33}}, \quad x_2 = \frac{1}{a_{22}}(b_2 - a_{23}x_3), \quad x_1 = \frac{1}{a_{11}}(b_1 - a_{12}x_2 - a_{13}x_3). \tag{20}$$

Gauss Elimination

The Gauss algorithm consists of a series of steps to bring any $n \times n$ matrix into the upper triangular form.

1. Sort the rows of A so that the diagonal coefficient a_{ii} (called *the pivot*) of row i (for all i) is non-zero. If this is not possible, the LSE cannot be solved.
2. Replace the j-th equation with

$$-\frac{a_{j1}}{a_{11}} \times (\text{1-st equation}) + (j\text{-th equation}) \; , \qquad (21)$$

   where j runs from 2 to n. This will zero-out column 1 for $i > 1$.

Gauss Elimination

3. Repeat the previous step, but starting with the next row down and with $j >$ (current row number). The current row be row k. Then we must replace rows j, $j > k$, with

$$-\frac{a_{jk}}{a_{kk}} \times (k\text{-th equation}) + (j\text{-th equation}) \,, \tag{22}$$

   where $k < j \leq n$.
4. Repeat (3) until all rows have been reduced and the matrix is in upper triangular form.
5. Back-substitute to find $\mathbf{x}$.

Gauss Elimination. Example

Consider the system

$$\begin{pmatrix} 5 & 3 & 4 \\ 2 & 1 & 5 \\ 5 & 4 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 3 \\ 4 \\ 2 \end{pmatrix} . \tag{23}$$

1. The pivots a_{ii} are all non-zero.

Gauss Elimination. Example

2. Now we replace the second equation with

$$-\frac{a_{21}}{a_{11}} \times (\text{First equation}) + (\text{Second equation}), \tag{24}$$

which gives:

$$\begin{aligned}
-\frac{2}{5} \times (5x_1 + 3x_2 + 4x_3) + (2x_1 + x_2 + 5x_3) &= -\frac{2}{5} \times 3 + 4 \\
\left(-\frac{6}{5} + 1\right) x_2 + \left(-\frac{8}{5} + 5\right) x_3 &= -\frac{6}{5} + 4 \\
-\frac{1}{5} x_2 + \frac{17}{5} x_3 &= \frac{14}{5} \\
-x_2 + 17x_3 &= 14 \qquad (25)
\end{aligned}$$

Gauss Elimination. Example

Hence the system becomes

$$\begin{pmatrix} 5 & 3 & 4 \\ 0 & -1 & 17 \\ 5 & 4 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 3 \\ 14 \\ 2 \end{pmatrix} . \tag{26}$$

Gauss Elimination. Example

2. Similarly, the third equation is replaced by

$$-\frac{a_{31}}{a_{11}} \times (\text{First equation}) + (\text{Third equation}), \qquad (27)$$

which gives

$$\begin{aligned} -\frac{5}{5} \times (5x_1 + 3x_2 + 4x_3) + (5x_1 + 4x_2 + x_3) &= -\frac{5}{5} \times 3 + 2 \\ \left(-\frac{15}{5} + 4\right) x_2 + \left(-\frac{20}{5} + 1\right) x_3 &= -3 + 2 \\ x_2 - 3x_3 &= -1 \qquad (28) \end{aligned}$$

Gauss Elimination. Example

The system is now

$$\begin{pmatrix} 5 & 3 & 4 \\ 0 & -1 & 17 \\ 0 & 1 & -3 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 3 \\ 14 \\ -1 \end{pmatrix} . \tag{29}$$

Gauss Elimination. Example

3. Now the third equation is replaced by the expression

$$-\frac{a_{32}}{a_{22}} \times (\text{Second equation}) + (\text{Third equation}), \tag{30}$$

which gives

$$\begin{aligned} -\frac{1}{-1} \times (-x_2 + 17x_3) + (x_2 - 3x_3) &= -\frac{1}{-1} \times 14 + (-1) \\ (-1+1)\, x_2 + (17-3)\, x_3 &= 14 - 1 \\ 14x_3 &= 13 \end{aligned} \tag{31}$$

Gauss Elimination. Example

The diagonalized system is finally

$$\begin{pmatrix} 5 & 3 & 4 \\ 0 & -1 & 17 \\ 0 & 0 & 14 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 3 \\ 14 \\ 13 \end{pmatrix} . \tag{32}$$

Gauss Elimination. Example

Back substitution gives

$$x_3 = \frac{13}{14} \tag{33}$$

$$x_2 = 17x_3 - 14 = 17\frac{13}{14} - 14 = \frac{25}{14} \tag{34}$$

$$x_1 = \frac{1}{5}\left(-3x_2 - 4x_3 + 3\right) = \frac{1}{5}\left(-3\frac{25}{14} - 4\frac{13}{14} + 3\right) = -\frac{17}{14} \tag{35}$$

Decomposition Methods (LU Decomposition)

Decomposition methods want to split a given LSE into smaller, considerably easier to solve parts.
The simplest such method is the Lower-Upper (LU) decomposition.

Given $A\mathbf{x} = \mathbf{b}$, suppose we can write the matrix A as

$$A = LU \ , \tag{36}$$

where L is lower triangular and U is upper triangular.

Decomposition Methods (LU Decomposition)

The solution of the LSE becomes

$$A\mathbf{x} = \mathbf{b} \longrightarrow (LU)\mathbf{x} = \mathbf{b} \longrightarrow L(U\mathbf{x}) = \mathbf{b} \ . \tag{37}$$

Defining $\mathbf{y} = U\mathbf{x}$, the original system is transformed into two systems

$$\begin{aligned} (1) \quad & L\mathbf{y} = \mathbf{b} \ , \\ (2) \quad & U\mathbf{x} = \mathbf{y} \ . \end{aligned} \tag{38}$$

Both these LSEs are triangular. (1) can be trivially solved by forward-substitution and (2) can be trivially solved by back-substitution.
The difficult part is now to find the L and U parts of A! This is done via matrix factorization.

Factorization of a Matrix

The process of decomposing A into L and U parts is called factorization. This decomposition is not generally unique and there are multiple ways of factorizing A.

A is an $n \times n$ matrix with n^2 coefficients. L and U are triangular and have $n(n+1)/2$ entries each for a total of $n^2 + n$ entries. Hence, L and U together have n coefficients more than A and these can be chosen to our own liking.

To derive the LU factorization, we begin by writing out $A = LU$ in coefficients:

$$a_{ij} = \sum_{s=1}^{n} l_{is} u_{sj} = \sum_{s=1}^{\min(i,j)} l_{is} u_{sj} \ , \tag{39}$$

where we have used that $l_{is} = 0$ for $s > i$ and $u_{sj} = 0$ for $s > j$.

Factorization of a Matrix

Let's start with entry $a_{ij} = a_{11}$:

$$a_{11} = l_{11} u_{11} \ . \tag{40}$$

We can now make use of the freedom of choosing n coefficients of L and U.
In *Doolittle's factorization*, one sets $l_{ii} = 1$, which makes L *unit triangular*.
In *Crout's factorization*, one sets $u_{ii} = 1$, which means that U is unit triangular.

Factorization of a Matrix

Following Doolittle, we set $l_{11} = 1$ and, with this, $u_{11} = a_{11}$. We can now compute all the elements of the first row of U and of the first column of L by setting $i = 1$ or $j = 1$,

$$\begin{aligned} u_{1j} &= a_{1j} \qquad i = 1, j > 1 \ , \\ l_{i1} &= \frac{a_{i1}}{u_{11}} \qquad j = 1, i > 1 \ . \end{aligned} \tag{41}$$

Factorization of a Matrix

Consider now a_{22}:

$$a_{22} = l_{21} u_{12} + l_{22} u_2 2 \; . \tag{42}$$

With Doolittle, $l_{22} = 1$, thus $u_{22} = a_{22} - l_{21} u_{12}$, where u_{12} and l_{21} are known from the previous steps. The second row of U and the second column of L are now calculated by setting either $i = 2$ or $j = 2$:

$$\begin{aligned} u_{2j} &= a_{2j} - l_{21} u_{1j} \quad i = 2, j > 2 \; , \\ l_{i2} &= \frac{a_{i2} - l_{i1} u_{12}}{u_{22}} \quad j = 2, i > 2 \; . \end{aligned} \tag{43}$$

Factorization of a Matrix

This procedure can be repeated for all the rows and columns of U and L. In the following, we provide a compact form of the algorithm in pseudocode.

Factorization of a Matrix

For $k = 1, 2, \cdots, n$ do

- Choose either l_{kk} (Doolittle) or u_{kk} (Crout) [the choice must be non-zero] and compute the other from

$$l_{kk} u_{kk} = a_{kk} - \sum_{s=1}^{k-1} l_{ks} u_{sk} \ . \tag{44}$$

- Build the k-th row of U:
  For $j = k+1, \cdots, n$ do:

$$u_{kj} = \frac{1}{l_{kk}} \left(a_{kj} - \sum_{s=1}^{k-1} l_{ks} u_{sj} \right) \ . \tag{45}$$

- Build the k-th column of L:
  For $i = k+1, \cdots, n$ do:

$$l_{ik} = \frac{1}{u_{kk}} \left(a_{ik} - \sum_{s=1}^{k-1} l_{is} u_{sk} \right) \ . \tag{46}$$

Next Class

Ordinary Differential Equations