Computational Physics

Solving Linear Systems of Equations

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Introduction

In many instances we need to solve $\mathbf{A} \cdot \mathbf{x} = \mathbf{b}$, where

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1N} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2N} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3N} \\ & & & \vdots & \\ a_{N1} & a_{N2} & a_{N3} & \cdots & a_{NN} \end{pmatrix} \quad \mathbf{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_N \end{pmatrix} \quad \mathbf{b} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_N \end{pmatrix}$$

This requires

- Finding $\mathbf{A}^{-1}$, the inverse of the matrix
- Computing the determinant of a matrix $\mathbf{A}$
- The eigenvalues and eigenvectors of a matrix $\mathbf{A}$. That is, $\mathbf{A} \cdot \mathbf{v} = \lambda \mathbf{v}$,

Gauss Elimination Method

Consider $\mathbf{A} \cdot \mathbf{x} = \mathbf{b}$ with $\mathbf{A}$ a $N \times N$ matrix with $\det(\mathbf{A}) \neq 0$. That is,

$$\begin{aligned}
a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \ldots + a_{1N}x_N &= b_1 \\
a_{21}x_1 + a_{22}x_2 + a_{23}x_3 + \ldots + a_{2N}x_N &= b_2 \\
a_{31}x_1 + a_{32}x_2 + a_{33}x_3 + \ldots + a_{3N}x_N &= b_3 \\
&\vdots \\
a_{N1}x_1 + a_{N2}x_2 + a_{N3}x_3 + \ldots + a_{NN}x_N &= b_N
\end{aligned}$$

We will try to transform it into an upper-triangular linear system.

$$\begin{array}{cccccc}
\hat{a}_{11}x_1 & +\hat{a}_{12}x_2 & +\hat{a}_{13}x_3 & +\ldots & +\hat{a}_{1N}x_N & =\hat{b}_1 \\
0 & +\hat{a}_{22}x_2 & +\hat{a}_{23}x_3 & +\ldots & +\hat{a}_{2N}x_N & =\hat{b}_2 \\
0 & +0 & +\hat{a}_{33}x_3 & +\ldots & +\hat{a}_{3N}x_N & =\hat{b}_3 \\
 & & & \vdots & & \\
0 & +0 & +0 & +\ldots & +\hat{a}_{NN}x_N & =\hat{b}_N
\end{array}$$

Given

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1N} \\ a_{21} & a_{22} & a_{23} & \cdots & a_{2N} \\ a_{31} & a_{32} & a_{33} & \cdots & a_{3N} \\ & & & \vdots & \\ a_{N1} & a_{N2} & a_{N3} & \cdots & a_{NN} \end{pmatrix}$$

construct

$$\mathbf{M}_1 = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 \\ -\frac{a_{21}}{a_{11}} & 1 & 0 & \cdots & 0 \\ -\frac{a_{31}}{a_{11}} & 0 & 1 & \cdots & 0 \\ & & & \vdots & \\ -\frac{a_{N1}}{a_{11}} & 0 & 0 & \cdots & 1 \end{pmatrix}$$

and compute $\mathbf{M}_1\mathbf{A} \cdot \mathbf{x} = \mathbf{M}_1\mathbf{b}$

where

$$\mathbf{M}_1\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1N} \\ 0 & a_{22} - \frac{a_{21}}{a_{11}} a_{12} & a_{23} - \frac{a_{21}}{a_{11}} a_{13} & \cdots & a_{2N} - \frac{a_{21}}{a_{11}} a_{1N} \\ 0 & a_{32} - \frac{a_{31}}{a_{11}} a_{12} & a_{33} - \frac{a_{31}}{a_{11}} a_{13} & \cdots & a_{3N} - \frac{a_{31}}{a_{11}} a_{1N} \\ & & & \vdots & \\ 0 & a_{N2} - \frac{a_{N1}}{a_{11}} a_{12} & a_{N3} - \frac{a_{N1}}{a_{11}} a_{13} & \cdots & a_{NN} - \frac{a_{N1}}{a_{11}} a_{1N} \end{pmatrix}$$

$$\mathbf{M}_1\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1N} \\ 0 & a_{22}{}^{(1)} & a_{23}{}^{(1)} & \cdots & a_{2N}{}^{(1)} \\ 0 & a_{32}{}^{(1)} & a_{33}{}^{(1)} & \cdots & a_{3N}{}^{(1)} \\ & & & \vdots & \\ 0 & a_{N2}{}^{(1)} & a_{N3}{}^{(1)} & \cdots & a_{NN}{}^{(1)} \end{pmatrix}$$

and

$$\mathbf{M}_1\mathbf{b} = \begin{pmatrix} b_1 \\ b_2 - \frac{a_{21}}{a_{11}} b_1 \\ b_3 - \frac{a_{31}}{a_{11}} b_1 \\ \vdots \\ b_N - \frac{a_{N1}}{a_{11}} b_1 \end{pmatrix} = \begin{pmatrix} b_1{}^{(1)} \\ b_2{}^{(1)} \\ b_3{}^{(1)} \\ \vdots \\ b_N{}^{(1)} \end{pmatrix}$$

The procedure can be repited to eliminate now $a_{32}{}^{(1)}$

Gauss Method

After $N-1$ steps we get the the desired upper-triangular system:

$$\begin{aligned}
a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \cdots + a_{1N}x_N &= b_1 \\
a_{22}^{(1)}x_2 + a_{23}^{(1)}x_3 + \cdots + a_{2N}^{(1)}x_N &= b_2^{(1)} \\
a_{33}^{(2)}x_3 + \cdots + a_{3N}^{(2)}x_N &= b_3^{(2)} \\
&\vdots \\
a_{NN}^{(N-1)}x_N &= b_N^{(N-1)}
\end{aligned}$$

The Nth (last) equation above yields :

$$x_N = \frac{b_N^{(N-1)}}{a_{NN}^{(N-1)}} \quad \text{for} \quad a_{NN}^{(N-1)} \neq 0$$

while the rest of the values can be calculated via the relation:

$$x_i = \frac{b_i^{(i-1)} - \sum_{k=i+1}^{N} a_{ik}^{(i-1)} x_k}{a_{ii}^{(i-1)}} \quad \text{for} \quad a_{ii}^{(i-1)} \neq 0$$

- The number of arithmetic operations needed is $(4N^3 + 9N^2 - 7N)/6$.
- If a matrix is transformed into an upper-triangular or lower-triangular or diagonal form then the determinant is simply

$$\det \mathbf{A} = a_{11} \cdot a_{22} \cdot a_{33} \cdots a_{NN} = \prod_{i=1}^{N} a_{ii}$$

Pivoting

Notice that there is trouble when $a_{ii}^{(i-1)} = 0$

$$x_i = \frac{b_i^{(i-1)} - \sum_{k=i+1}^{N} a_{ik}^{(i-1)} x_k}{a_{ii}^{(i-1)}} \quad \text{for} \quad a_{ii}^{(i-1)} \neq 0$$

The number a_{ii} in the position (i, i) that is used to eliminate x_i in rows $i+1$, $i+2$, ... ,N is called the ith **pivotal element** and the ith row is called the **pivotal row**.

If $a_{ii}^{(i)} = 0$, row i cannot be used to eliminate, the elements in column i below the diagonal. It is neccesary to find a row j, where $a_{ji}^{(i)} \neq 0$ and $j > i$ and then interchange row i and j so that a nonzero pivot element is obtained.

The Jacobi Method

Any system of N linear equations with N unknowns can be written in the form:

$$
\begin{aligned}
f_1(x_1, x_2, ..., x_N) &= 0 \\
f_2(x_1, x_2, ..., x_N) &= 0 \\
&\;.....\\
f_n(x_1, x_2, ..., x_N) &= 0
\end{aligned}
$$

One can always rewrite the system in the form $x_i = g_i\left(x_j\right)$; that is,

$$
\begin{aligned}
x_1 &= g_1(x_2, x_3, ..., x_N) \\
x_2 &= g_2(x_1, x_3, ..., x_N) \\
& ... \\
x_N &= g_N(x_1, x_2, ..., x_{N-1})
\end{aligned}
$$

or

$$x_i = \frac{b_i}{a_{ii}} - \frac{1}{a_{ii}} \sum_{j=1\,,\,j\neq i}^{N} a_{ij} x_j$$

Therefore, by giving N initial guesses $x_1^{(0)}, x_2^{(0)}, \ldots, x_N^{(0)}$, we create the recurrence relation

$$x_i^{(k+1)} = g_i(x_1^{(k)}, ..., x_N^{(k)}) = \frac{b_i}{a_{ii}} - \frac{1}{a_{ii}} \sum_{j=1\,,\,j\neq i}^{N} a_{ij}\, x_j^{(k)}$$

which will converge to the solution of the system if:

$$|a_{ii}| > \sum_{j=1\,,\,j\neq i}^{N} |a_{ij}| \quad \text{(Diagonal dominat)}$$

independent on the choice of the initial values $x_1^{(0)}, x_2^{(0)}, \ldots, x_N^{(0)}$.
The recurrence relation can be written in a matrix form as:

$$\mathbf{x}^{(\mathbf{k}+1)} = \mathbf{D}^{-1}\mathbf{b} - \mathbf{D}^{-1}\,\mathbf{C}\,\mathbf{x}^{(\mathbf{k})}$$

where $\mathbf{A} = \mathbf{D} + \mathbf{C}$ with $\mathbf{D} = \text{diag}(\mathbf{A})$ and $\mathbf{C}$ all the rest.

Consider the following example

$$\begin{aligned} 4x - y + z &= 7 \\ 4x - 8y + z &= -21 \\ -2x + y + 5z &= 15 \end{aligned}$$

with solutions $x = 2,\ y = 4,\ z = 3$. Construct the recurrence relationships

$$\begin{aligned} x^{(k+1)} &= (7 + y^{(k)} - z^{(k)})/4 \\ y^{(k+1)} &= (21 + 4x^{(k)} + z^{(k)})/8 \\ z^{(k+1)} &= (15 + 2x^{(k)} - y^{(k)})/5 \end{aligned}$$

Starting with $(1, 2, 2)$, one gets

$$\begin{aligned} (1,2,2) \quad &\rightarrow (1.75, 3.375, 3) \quad \rightarrow (1.844, 3.875, 3.025) \\ \rightarrow (1.963, 3.925, 2.963) \quad &\rightarrow (1.991, 3.977, 3.0) \quad \rightarrow (1.994, 3.995, 3.001) \end{aligned}$$

I.e. with 5 iterations we reached the solution with 3 digits accuracy.

Gauss - Seidel Method

Recall the Jacobi method

$$x_i^{(k+1)} = \frac{1}{a_{ii}} \left(b_i - \sum_{j=1\,,\, j\neq i}^{N} a_{ij}\, x_j^{(k)} \right)$$

- With $(x_1^{(0)}, x_2^{(0)}, x_3^{(0)}, ..., x_N^{(0)})$,

$$x_1^{(1)} = \frac{1}{a_{11}} \left(b_1 \sum_{j=2}^{N} a_{1j}\, x_j^{(0)} \right)$$

- Next with $(x_1^{(1)}, x_2^{(0)}, x_3^{(0)}, ..., x_N^{(0)})$,

$$x_2^{(2)} = \frac{1}{a_{22}} \left(b_2 - a_{21}\, x^{(1)} - \sum_{j=3}^{N} a_{3j}\, x_j^{(0)} \right)$$

- Next with $(x_1^{(1)}, x_2^{(1)}, x_3^{(0)}, ..., x_N^{(0)})$, and so on.

Recurrence relation:

$$
\begin{aligned}
x_1^{(k+1)} &= \frac{1}{a_{11}}\left(b_1 - \sum_{j=2}^{N} a_{1j}x_j^{(k)}\right) \\
x_2^{(k+1)} &= \frac{1}{a_{22}}\left(b_2 - a_{21}x_1^{(k+1)} - \sum_{j=3}^{N} a_{2j}x_j^{(k)}\right) \\
&\dots \\
x_i^{(k+1)} &= \frac{1}{a_{ii}}\left(b_i - \sum_{j=1}^{i-1} a_{ij}x_j^{(k+1)} - \sum_{j=i+1}^{N} a_{ij}x_j^{(k)}\right)
\end{aligned}
$$

The method will converge if:

$$|a_{ii}| > \sum_{j=1\,,\,j\neq i}^{N} |a_{ij}|$$

This procedure in a “matrix form” is:

$$\mathbf{x}^{(\mathbf{k+1})} = \mathbf{D}^{-1}\left[\mathbf{B} \;-\; \mathbf{L}\mathbf{x}^{(\mathbf{k+1})} - \mathbf{U}\mathbf{x}^{(\mathbf{k})}\right]$$

where

$$\mathbf{A} = \underset{lower}{\mathbf{L}} + \underset{diagonal}{\mathbf{D}} + \underset{upper}{\mathbf{U}}$$

The matrix **L** has the elements of below the diagonal **A**, the matrix **D** only the diagonal elements of **A** and finally the matrix **U** the elements of matrix **A** over the diagonal.

The recurrence relation for the previous example becomes in this case

$$\begin{aligned} x^{(k+1)} &= \frac{7 + y^{(k)} - z^{(k)}}{4} \\ y^{(k+1)} &= \frac{21 + 4x^{(k+1)} + z^{(k)}}{8} \\ z^{(k+1)} &= \frac{15 + 2x^{(k+1)} - y^{(k+1)}}{5} \end{aligned}$$

leading to the following sequence of approximate solutions:

$$\begin{aligned} (1, 2, 2) &\rightarrow (1.75, 3.75, 2, 95) \\ &\rightarrow (1.95, 3.97, 2.99) \\ &\rightarrow (1.996, 3.996, 2.999) \end{aligned}$$

i.e. here we need only 3 iterations to arrive to the same accuracy of solutions as with Jacobi's method which needed 5 iterations.

Eigenvalues and Eigenvectors

Given a matrix $\mathbf{A}$, if there exist a scalar λ and vector $\mathbf{u}$ such that

$$\mathbf{A} \cdot \mathbf{u} = \lambda \, \mathbf{u}$$

λ is called an eigenvalue of the matrix $\mathbf{A}$ and $\mathbf{u}$ the corresponding eigenvector.

Example:

$$\underbrace{\begin{pmatrix} 1 & 2 & 3 \\ -1 & 3 & 1 \\ 2 & 0 & 1 \end{pmatrix}}_{\mathbf{A}} \cdot \underbrace{\begin{pmatrix} 2 \\ 1 \\ -2 \end{pmatrix}}_{\mathbf{u}^{(1)}} = \underbrace{-1}_{\lambda_1} \cdot \underbrace{\begin{pmatrix} 2 \\ 1 \\ -2 \end{pmatrix}}_{\mathbf{u}^{(1)}}$$

in which $\mathbf{u}^{(1)} = (2, 1, -2)^\top$ is the e-vector and $\lambda_1 = -1$ the corresponding e-value of $\mathbf{A}$.

Equation $\mathbf{A} \cdot \mathbf{u} = \lambda \, \mathbf{u}$ is equivalent to $\det(\mathbf{A} - \lambda \mathbf{I}) = 0$. That is

$$\det \begin{vmatrix} 1-\lambda & 2 & 3 \\ -1 & 3-\lambda & 1 \\ 2 & 0 & 1-\lambda \end{vmatrix} = \lambda^3 - 5\lambda^2 + 3\lambda + 9 = 0$$

and the e-values will be the roots of the characteristic polynomial (here $\lambda_i = -1$, 3 and 3).

Given a matrix $\mathbf{A}$, such that

$$\mathbf{A}\,\mathbf{u}^{(i)} = \lambda_i \mathbf{u}^{(i)}\,, \qquad (1 \le i \le N)$$

there will always be a dominant e-value λ_1. That is,

$$|\lambda_1| \ge |\lambda_2| \ge |\lambda_3| \ge \ldots \ge |\lambda_N|$$

In addition, any vector $\vec{x}$ can be written as a linear combination of the N e-vectors $\left\{\mathbf{u}^{(1)}, \mathbf{u}^{(2)}, \ldots, \mathbf{u}^{(N)}\right\}$. That is,

$$\mathbf{x} = a_1 \mathbf{u}^{(1)} + a_2 \mathbf{u}^{(2)} + \cdots + a_N \mathbf{u}^{(N)}$$

Consider

$$\begin{aligned}\mathbf{x}^{(k)} &\equiv \mathbf{A}^k \cdot \mathbf{x} = a_1 \lambda_1^k \mathbf{u}^{(1)} + a_2 \lambda_2^k \mathbf{u}^{(2)} + \cdots + a_N \lambda_N^k \mathbf{u}^{(N)} \\ &= \lambda_1^k \left[a_1 \mathbf{u}^{(1)} + a_2 \left(\frac{\lambda_2}{\lambda_1}\right)^k \mathbf{u}^{(2)} + \cdots + a_N \left(\frac{\lambda_N}{\lambda_1}\right)^k \mathbf{u}^{(N)} \right]\end{aligned}$$

Since λ_1 is the absolute largest e-value, $\lim_{k\to\infty} \left(\lambda_j/\lambda_1\right)^k = 0$. Thus, for a large enough k, we have that

$$\mathbf{x}^{(k)} = \mathbf{A}^k \cdot \mathbf{x} \approx \lambda_1^k \, a_1 \, \mathbf{u}^{(1)}$$

and in particular

$$\mathbf{x}^{(k+1)} = \lambda_1 \, \mathbf{x}^{(k)}$$

Therefore, for each component of the vectors $\mathbf{x}^{(k)}$ and $\mathbf{x}^{(k+1)}$, we have that

$$\frac{[\mathbf{x}^{(k+1)}]_a}{[\mathbf{x}^{(k)}]_a} = \lambda_1$$

Example:

$$\mathbf{A} = \begin{pmatrix} 1 & 0 & 1 \\ -1 & 2 & 2 \\ 1 & 0 & 3 \end{pmatrix}$$

with e-values:

$$\begin{aligned} \lambda_1 &= 3.41421356 \\ \lambda_2 &= 2 \\ \lambda_3 &= 0.585786 \end{aligned}$$

and corresponding e-vectors :

$$\begin{aligned} \mathbf{u}^{(1)} &= (0.3694,\ 1,\ 0.8918)^\top \\ \mathbf{u}^{(2)} &= (0,\ 1,\ 0)^\top \\ \mathbf{u}^{(3)} &= (0.7735,\ 1,\ -0.3204)^\top \end{aligned}$$

Set $\mathbf{x} = (1, 2, 1)^\top$, and multiply it with the 5th and 6th power of $\mathbf{A}$

$$\mathbf{A}^5 = \begin{pmatrix} 68 & 0 & 164 \\ 136 & 32 & 428 \\ 164 & 0 & 396 \end{pmatrix} \quad \mathbf{A}^6 = \begin{pmatrix} 232 & 0 & 560 \\ 532 & 64 & 1484 \\ 560 & 0 & 1352 \end{pmatrix}$$

Thus,

$$\begin{aligned} \mathbf{x}^{(5)} &= \mathbf{A}^5 \cdot \mathbf{x} = (232, 628, 560)^\top \\ \mathbf{x}^{(6)} &= \mathbf{A}^6 \cdot \mathbf{x} = (792, 2144, 1912)^\top \end{aligned}$$

which yields

$$\lambda_1 \approx \frac{[\mathbf{x}^{(6)}]_a}{[\mathbf{x}^{(5)}]_a} = \frac{792}{232} \approx \frac{2144}{628} \approx \frac{1912}{560} \approx 3.414286$$