Computational Physics

Solving Linear Systems of Equations

Lectures based on course notes by Pablo Laguna and Kostas Kokkotas

revamped by Deirdre Shoemaker

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Gauss Method

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

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

We can solve for the x_N

The Nth (last) equation above yields :

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

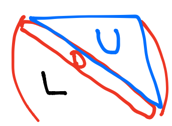
now we can head back ↑

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 $a_{ii}^{(i-1)} = 0$

we can rewrite our matrix such that it is non-singular

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

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.

But: This method accumulate error, especially large N
Iterative ↓

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

faster but need a good guess

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

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:

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

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

$$\left(D \right) x^{new} + \left(L \quad U \right) x^{old} = b$$

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

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

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

Gauss - Seidel Method

Recall the Jacobi method

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

More efficient: when computing x^{new} at k, use $k-1$ (x^{old}) this speeds up convergence

- 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:

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

The method will converge if:

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

$\begin{pmatrix} L \;\; D \end{pmatrix} x^{new} + \begin{pmatrix} U \end{pmatrix} x^{old} = b$

This procedure in a “matrix form” is:

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

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.