Numerical Analysis IV: solving linear systems

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Two different approaches

Solve $Ax = b$

Direct methods:

- Deterministic
- Exact up to machine precision
- Expensive (in time and space)

Iterative methods:

- Only approximate
- Cheaper in space and (possibly) time
- Convergence not guaranteed

Really bad example of direct method

Cramer's rule
write $|A|$ for determinant, then

$$x_i = \begin{vmatrix} a_{11} & a_{12} & \ldots & a_{1i-1} & b_1 & a_{1i+1} & \ldots & a_{1n} \\ a_{21} & & \ldots & & b_2 & & \ldots & a_{2n} \\ \vdots & & & & \vdots & & & \vdots \\ a_{n1} & & \ldots & & b_n & & \ldots & a_{nn} \end{vmatrix} / |A|$$

Time complexity $O(n!)$

Gaussian elimination

Example

$$\begin{pmatrix} 6 & -2 & 2 \\ 12 & -8 & 6 \\ 3 & -13 & 3 \end{pmatrix} x = \begin{pmatrix} 16 \\ 26 \\ -19 \end{pmatrix}$$

$$\left[\begin{array}{ccccc} 6 & -2 & 2 & | & 16 \\ 12 & -8 & 6 & | & 26 \\ 3 & -13 & 3 & | & -19 \end{array}\right] \longrightarrow \left[\begin{array}{ccccc} 6 & -2 & 2 & | & 16 \\ 0 & -4 & 2 & | & -6 \\ 0 & -12 & 2 & | & -27 \end{array}\right] \longrightarrow \left[\begin{array}{ccccc} 6 & -2 & 2 & | & 16 \\ 0 & -4 & 2 & | & -6 \\ 0 & 0 & -4 & | & -9 \end{array}\right]$$

Solve x_3, then x_2, then x_1

$6, -4, -4$ are the 'pivots'

Pivoting

If a pivot is zero, exchange that row and another.
(there is always a row with a nonzero pivot if the matrix is nonsingular)
best choice is the largest possible pivot
in fact, that's a good choice even if the pivot is not zero

Roundoff control

Consider

$$\begin{pmatrix} \epsilon & 1 \\ 1 & 1 \end{pmatrix} x = \begin{pmatrix} 1+\epsilon \\ 2 \end{pmatrix}$$

with solution $x = (1,1)^t$

Ordinary elimination:

$$\begin{pmatrix} \epsilon & 1 \\ 0 & (1-\frac{1}{\epsilon}) \end{pmatrix} x = \begin{pmatrix} 1 \\ 2-\frac{1}{\epsilon} \end{pmatrix}$$

$$\Rightarrow x_2 = \frac{2-\frac{1}{\epsilon}}{1-\frac{1}{\epsilon}} \Rightarrow x_1 = \frac{1-x_2}{\epsilon}$$

Roundoff 2

If $\epsilon < \epsilon_{\mathrm{mach}}$, then $2 - 1/\epsilon = -1/\epsilon$ and $1 - 1/\epsilon = -1/\epsilon$, so

$$x_2 = \frac{2 - \frac{1}{\epsilon}}{1 - \frac{1}{\epsilon}} = 1, \Rightarrow x_1 = \frac{1 - x_2}{\epsilon} = 0$$

Roundoff 3

Pivot first:

$$\begin{pmatrix}1 & 1\\ \epsilon & 1\end{pmatrix} x = \begin{pmatrix}2\\1\end{pmatrix} \Rightarrow \begin{pmatrix}1 & 1\\ 0 & 1-\epsilon\end{pmatrix} x = \begin{pmatrix}2\\ 1-2\epsilon\end{pmatrix}$$

If ϵ very small:

$$x_1 = \frac{1-2\epsilon}{1-\epsilon} = 1, \qquad x_2 = 2 - x_1 = 1$$

LU factorization

Same example again:

$$A = \begin{pmatrix} 6 & -2 & 2 \\ 12 & -8 & 6 \\ 3 & -13 & 3 \end{pmatrix}$$

2nd row minus $2\times$ first; 3rd row minus $1/2\times$ first; equivalent to

$$L_1 A x = L_1 b, \qquad L_1 = \begin{pmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ -1/2 & 0 & 1 \end{pmatrix}$$

LU 2

Next step: $L_2 L_1 A x = L_2 L_1 b$ with

$$L_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -3 & 1 \end{pmatrix}$$

Define $U = L_2 L_1 A$, then $A = L_1^{-1} L_2^{-1} U$
'LU factorization'

LU 3

Observe:

$$L_1 = \begin{pmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ -1/2 & 0 & 1 \end{pmatrix} \qquad L_1^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 1/2 & 0 & 1 \end{pmatrix}$$

Likewise

$$L_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -3 & 1 \end{pmatrix} \qquad L_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 3 & 1 \end{pmatrix}$$

Even more remarkable:

$$L_1^{-1} L_2^{-1} = \begin{pmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 1/2 & 3 & 1 \end{pmatrix}$$

Can be computed in place! (pivoting?)

Solve LU system

$Ax = b \longrightarrow LUx = b$ solve in two steps:
$Ly = b$, and $Ux = y$

Forward sweep:

$$\begin{pmatrix} 1 & & & \emptyset & \\ \ell_{21} & 1 & & & \\ \ell_{31} & \ell_{32} & 1 & & \\ \vdots & & \ddots & & \\ \ell_{n1} & \ell_{n2} & & \cdots & 1 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ \\ \vdots \\ y_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ \\ \vdots \\ b_n \end{pmatrix}$$

$$y_1 = b_1, \quad y_2 = b_2 - \ell_{21} y_1, \ldots$$

Solve LU 2

Backward sweep:

$$\begin{pmatrix} u_{11} & u_{12} & \ldots & u_{1n} \\ & u_{22} & \ldots & u_{2n} \\ & & \ddots & \vdots \\ \emptyset & & u_{nn} & \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}$$

$$x_n = u_{nn}^{-1} y_n, \quad x_{n-1} = u_{n-1n-1}^{-1}(y_{n-1} - u_{n-1n}x_n), \ldots$$

Sparsity patterns

One-dimensional boundary value problem: tri-diagonal matrix

Sparsity pattern of $L + U$ is the same as of A. This is not typical.

Two/three dimensional boundary value problems

$$-u_{xx} - u_{yy} = f$$

banded matrices

Domain Ω of $n \times n$ points:
$\Rightarrow$ matrix A of $N \times N$ points, where $N = n^2$

Matrix has 5-diagonal (penta-diagonal) structure: diagonals at distance of ± 1, $\pm n$ from the main diagonal

The fill-in phenomenon

Elementary fact: LU factorization of a banded matrix gives ‘fill-in’ inside the band

Iterative methods

Choose any x_0 and repeat

$$x^{k+1} = Bx^k + c$$

until $\|x^{k+1} - x^k\|_2 < \epsilon$ or until $\frac{\|x^{k+1}-x^k\|_2}{\|x^k\|} < \epsilon$

Example of iterative solution

Example system

$$\begin{pmatrix} 10 & 0 & 1 \\ 1/2 & 7 & 1 \\ 1 & 0 & 6 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 21 \\ 9 \\ 8 \end{pmatrix}$$

with solution $(2, 1, 1)$.

Suppose you know (physics) that solution components are roughly the same size, and observe the dominant size of the diagonal, then

$$\begin{pmatrix} 10 & & \\ & 7 & \\ & & 6 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 21 \\ 9 \\ 8 \end{pmatrix}$$

might be a good approximation: solution $(2.1, 9/7, 8/6)$.

Iterative example′

Example system

$$\begin{pmatrix} 10 & 0 & 1 \\ 1/2 & 7 & 1 \\ 1 & 0 & 6 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 21 \\ 9 \\ 8 \end{pmatrix}$$

with solution $(2, 1, 1)$.

Also easy to solve:

$$\begin{pmatrix} 10 & & \\ 1/2 & 7 & \\ 1 & 0 & 6 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} 21 \\ 9 \\ 8 \end{pmatrix}$$

with solution $(2.1, 7.95/7, 5.9/6)$.

Iterative example''

Instead of solving $Ax = b$ we solved $L\tilde{x} = b$. Look for the missing part: $x = \tilde{x} + \Delta x$, then $A\Delta x = b - A\tilde{x} \equiv r$. Solve again $L\widetilde{\Delta x} = r$ and update $\tilde{\tilde{x}} = \tilde{x} + \widetilde{\Delta x}$.

iteration	1	2	3
x_1	2.1000	2.0017	2.000028
x_2	1.1357	1.0023	1.000038
x_3	0.9833	0.9997	0.999995

Two decimals per iteration. *This is not typical*

Exact system solving: $O(n^3)$ cost; iteration: $O(n^2)$ per iteration. Potentially cheaper if the number of iterations is low.

Abstract presentation

- To solve $Ax = b$; too expensive; suppose $K \approx A$ and solving $Kx = b$ is possible
- Define $Kx_0 = b$, then error correction $e_0 = x - x_0$, and $A(x_0 + e_0) = b$
- so $Ae_0 = b - Ax_0 = r_0$; this is again unsolvable, so
- $K\tilde{e}_0$ and $x_1 = x_0 + \tilde{e}_0$.
- now iterate: $e_1 = x - x_1$, $Ae_1 = b - Ax_1 = r_1$ et cetera

Error analysis

- One step

$$
\begin{aligned}
r_1 &= b - Ax_1 = b - A(x_0 + \tilde{e}_0) && (1)\\
&= r_0 - AK^{-1}r_0 && (2)\\
&= (I - AK^{-1})r_0 && (3)
\end{aligned}
$$

- Inductively: $r_n = (I - AK^{-1})^n r_0$ so $r_n \downarrow 0$ if $|\lambda(I - AK^{-1})| < 1$
  Geometric reduction (or amplification!)
- This is 'stationary iteration': every iteration step the same.
  Simple analysis, limited applicability.

Choice of K

- The closer K is to A, the faster convergence.
- Diagonal and lower triangular choice mentioned above: let

$$A = D_A + L_A + U_A$$

  be a splitting into diagonal, lower triangular, upper triangular part, then
- Jacobi method: $K = D_A$ (diagonal part),
- Gauss-Seidel method: $K = D_A + L_A$ (lower triangle, including diagonal)

Choice of K through incomplete LU

- Inspiration from direct methods: let $K = LU \approx A$

Gauss elimination:

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for k,i,j:
   a[i,j] = a[i,j] - a[i,k] * a[k,j] / a[k,k]
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Incomplete variant:

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for k,i,j:
  if a[i,j] not zero:
    a[i,j] = a[i,j] - a[i,k] * a[k,j] / a[k,k]
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$\Rightarrow$ sparsity of $L + U$ the same as of A

Stopping tests

When to stop converging? Can size of the error be guaranteed?

- Direct tests on error $e_n = x - x_n$ impossible; two choices
- Relative change in the computed solution small:

$$\|x_{n+1} - x_n\| / \|x_n\| < \epsilon$$

- Residual small enough:

$$\|r_n\| = \|Ax_n - b\| < \epsilon$$

Without proof: both imply that the error is less than some other ϵ'.

General iterative methods

- Residual calculation: matrix-vector product
- Solve system with matrix close to A
- Some vector operations (including inner products, in general)