Gaussian Elimination

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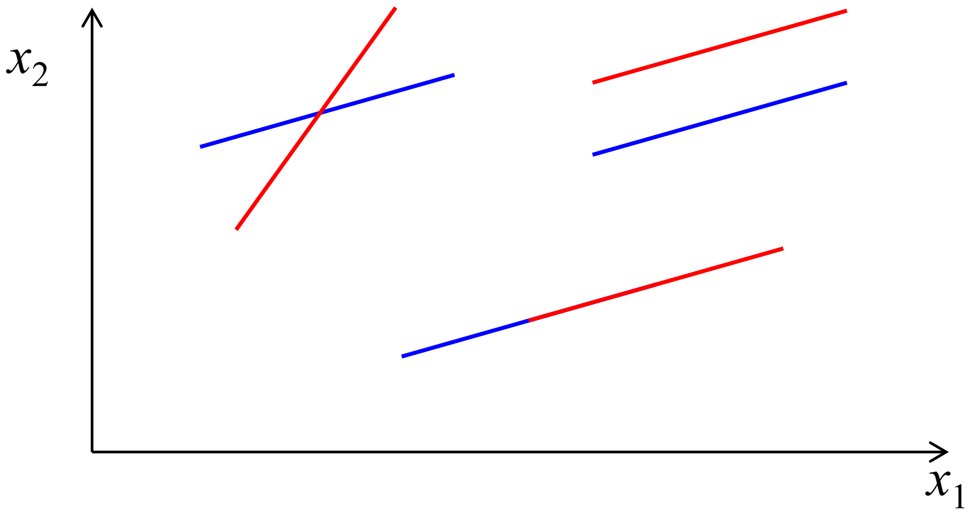
Overview

- Explicit Solutions
- Determinants
- Gauss Elimination
- LU Decomposition
- Pivoting
- Scaling
- Backward Error Analysis

Two Linear Equations

$$\begin{cases} a_{11}x_1 + a_{12}x_2 = b_1 \\ a_{21}x_1 + a_{22}x_2 = b_2 \end{cases} \qquad \mathbf{Ax} = \mathbf{b} \qquad \mathbf{Ax} = \mathbf{0}$$



Cramer's Rule, 1750

$$\begin{cases} a_{11}x_1 + a_{12}x_2 = b_1 \\ a_{21}x_1 + a_{22}x_2 = b_2 \end{cases}$$

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

$$x_1 = \frac{\begin{vmatrix} b_1 & a_{12} \\ b_2 & a_{22} \end{vmatrix}}{\begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix}}; \qquad x_2 = \frac{\begin{vmatrix} a_{11} & b_1 \\ a_{21} & b_2 \end{vmatrix}}{\begin{vmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{vmatrix}}.$$

$$x_i = \frac{\det(\mathbf{A}_i)}{\det(\mathbf{A})}$$

Determinant

$$\det\left(\mathbf{A}\right)=\sum_{\sigma}(-1)^{\sigma}a_{1\sigma_1}a_{2\sigma_2}\dots a_{n\sigma_n}$$

$$\begin{array}{ccccc} a_{11} & a_{12} & a_{13} & a_{11} & a_{12} \\ a_{21} & a_{22} & a_{12} & a_{21} & a_{22} \\ a_{31} & a_{32} & a_{13} & a_{31} & a_{32} \end{array}$$

$$10!=3,628,800 \qquad 100!\approx 10^{158}$$

170! is the largest factorial that can be approximated in 64-bit format.

Some Properties

$$\det\left(\mathbf{A}\right) = \sum_{i=1}^{n} (-1)^{i+j} a_{i,j} M_{i,j} = \sum_{j=1}^{n} (-1)^{i+j} a_{i,j} M_{i,j}$$

$$\det\left(\mathbf{I}\right) = 1$$

$$\det\left(\mathbf{AB}\right) = \det\left(\mathbf{A}\right)\det\left(\mathbf{B}\right) \longrightarrow \det\left(\mathbf{A}^{-1}\right) = 1/\det\left(\mathbf{A}\right)$$

$$\det\left(\mathbf{A}^{T}\right) = \det\left(\mathbf{A}\right)$$

$$\det\left(\alpha\mathbf{A}\right) = \alpha^{n}\det\left(\mathbf{A}\right)$$

Singular Matrix Indicator

$$\mathbf{A}\mathbf{x} = \mathbf{b} \qquad \det\left(\mathbf{A}\right) = 0 \qquad \det\left(\mathbf{A}\right) \approx 0$$

In theory　　In Practice

$$\mathbf{A} = \begin{bmatrix} 0.1 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 0.1 \end{bmatrix} \qquad 100 \times 100$$

$$\det\left(\mathbf{A}\right) = 10^{-100} \longleftrightarrow \kappa\left(\mathbf{A}\right) = ?$$

Naïve Gauss Elimination

$$\begin{cases} a_{11}x_1 + a_{12}x_2 + \ldots + a_{1n}x_n = b_1 & \mathcal{E}_1 \\ a_{21}x_1 + a_{22}x_2 + \ldots + a_{2n}x_n = b_2 & \mathcal{E}_2 \\ a_{31}x_1 + a_{32}x_2 + \ldots + a_{3n}x_n = b_3 & \mathcal{E}_3 \\ \qquad\qquad\vdots & \\ a_{n1}x_1 + a_{n2}x_2 + \ldots + a_{nn}x_n = b_n & \mathcal{E}_n \end{cases}$$

$$\mathcal{E}_2 \to \mathcal{E}_2 - \mathcal{E}_1 \frac{a_{2,1}}{a_{1,1}}: \quad a'_{22}x_2 + \ldots + a'_{2n}x_n = b'_2$$

$$\mathcal{E}_3 \to \mathcal{E}_3 - \mathcal{E}_1 \frac{a_{3,1}}{a_{1,1}}: \quad a'_{32}x_2 + \ldots + a'_{3n}x_n = b'_3$$

$\vdots$

Forward Elimination

$$\begin{cases} a_{11}x_1 + a_{12}x_2 + \ldots + a_{1n}x_n = b_1 \\ \qquad\quad a'_{22}x_2 + \ldots + a'_{2n}x_n = b'_2 \\ \qquad\qquad\qquad\qquad\qquad \vdots \\ \qquad\quad a'_{n2}x_2 + \ldots + a'_{nn}x_n = b'_n \end{cases}$$

$$\begin{cases} a_{11}x_1 + a_{12}x_2 + \ldots + a_{1n}x_n = b_1 \\ \qquad\quad a'_{22}x_2 + \ldots + a'_{2n}x_n = b'_2 \\ \qquad\qquad\qquad\qquad\qquad \vdots \\ \qquad\qquad\qquad\quad a_{nn}^{(n-1)}x_n = b_n^{(n-1)} \end{cases}$$

Backward Substitution

$$x_n = \frac{b_n^{(n-1)}}{a_{nn}^{(n-1)}}$$

$$x_i = \frac{b_i^{(i-1)} - \sum_{j=i+1}^{n} a_{ij}^{(i-1)} x_j}{a_{ii}^{(i-1)}}; \quad i = n-1, \ldots, 1$$

Totally about $2n^3/3$ arithmetic operations

- $n(n-1)/2$ divisions
- $(2n^3+3n^2-5n)/6$ multiplications
- $(2n^3+3n^2-5n)/6$ subtractions

Eliminating 1-st Column

$$\begin{bmatrix} 1 & 0 & \cdots & 0 \\ -a_{21}/a_{11} & 1 & \cdots & 0 \\ \vdots & 0 & \ddots & 0 \\ -a_{n1}/a_{11} & 0 & \cdots & 1 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \cdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & a'_{22} & \cdots & a'_{2n} \\ \vdots & \vdots & \cdots & \vdots \\ 0 & a'_{n2} & \cdots & a'_{nn} \end{bmatrix}$$

$$\mathbf{L}_1\mathbf{A} \equiv \mathbf{A}_1$$

$$\mathbf{L}_1\mathbf{A}\mathbf{x} = \mathbf{L}_1\mathbf{b}$$

LU-Factorisation

$$\mathbf{L}_2\mathbf{L}_1\mathbf{A}\mathbf{x} = \mathbf{L}_2\mathbf{L}_1\mathbf{b}$$

$$\mathbf{L}_{n-1}\cdots\mathbf{L}_1\mathbf{A}\mathbf{x} = \mathbf{L}_{n-1}\cdots\mathbf{L}_1\mathbf{b}$$

$$\mathbf{L}_{n-1}\cdots\mathbf{L}_1\mathbf{A} \equiv \mathbf{U}$$

$$\mathbf{A} = \left(\mathbf{L}_{n-1}\cdots\mathbf{L}_1\right)^{-1}\mathbf{U}$$

$$\mathbf{A} = \mathbf{L}\mathbf{U} \qquad \mathbf{L}_{i,i} = 1$$

Formal LU-Solution

$$\mathbf{LUx} = \mathbf{b} \qquad\qquad \mathbf{y} \equiv \mathbf{Ux}$$

Forward elimination $\quad \mathbf{Ly} = \mathbf{b}$

Back substitution $\quad \mathbf{Ux} = \mathbf{y}$

Pitfalls of GE

- Division by zero
- Round-off errors
- Ill-Conditioned equations

Rounding Errors

$$\begin{bmatrix} 10^{-5} & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$\begin{cases} x_1 = \dfrac{-1}{1-10^{-5}} \approx -1 \\ x_2 = \dfrac{1}{1-10^{-5}} \approx +1 \end{cases}$$

$$\begin{bmatrix} 10^{-5} & 1 \\ 0 & 1-10^{5} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ -10^{5} \end{bmatrix}$$

(4-digit arithmetic)

$$1-10^{5} \downarrow -10^{5} \longrightarrow x_2 = 1 \qquad 10^{-5} x_1 + x_2 = 1 \longrightarrow x_1 = 0$$

Ill-Conditioned Systems

$$\begin{bmatrix} 1.0 & 2.0 \\ 1.1 & 2.0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 10.0 \\ 10.4 \end{bmatrix} \longrightarrow \begin{matrix} x_1 = 4 \\ x_2 = 3 \end{matrix}$$

$$\begin{bmatrix} 1.0 & 2.0 \\ 1.05 & 2.0 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 10.0 \\ 10.4 \end{bmatrix} \longrightarrow \begin{matrix} x_1 = 8 \\ x_2 = 1 \end{matrix}$$

Pivoting

- Partial pivoting
- Full pivoting

$$\begin{bmatrix} 1 & 0 & \cdots & 0 \\ -a_{21}/a_{11} & 1 & \cdots & 0 \\ \vdots & 0 & \ddots & 0 \\ -a_{n1}/a_{11} & 0 & \cdots & 1 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \cdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ 0 & a'_{22} & \cdots & a'_{2n} \\ \vdots & \vdots & \cdots & \vdots \\ 0 & a'_{n2} & \cdots & a'_{nn} \end{bmatrix}$$

Major Improvements

- Preconditioning by row equilibration
- Preconditioning by column equilibration
- Partial/Full pivoting
- Preconditioning or scaling with each major step of the elimination procedure
- Iterative improvement at the end

Row Equilibration

$$r_i \equiv 1 \Big/ \max_{1 \le j \le n} \left| a_{ij} \right| \qquad \left(1 \le i \le n \right)$$

$$\sum_{j=1}^{n} a_{ij} x_j = b_i \longrightarrow \sum_{j=1}^{n} r_i a_{ij} x_j = r_i b_i$$

$$\mathbf{Ax} = \mathbf{b} \longrightarrow \mathbf{RAx} = \tilde{\mathbf{A}}\mathbf{x} = \mathbf{Rb}$$

$$\max_{1 \le j \le n} \left| \tilde{a}_{ij} \right| = 1 \qquad \left(1 \le i \le n \right)$$

Left Multiplication

$$\mathbf{R}\mathbf{A} = \tilde{\mathbf{A}}$$

$$\begin{bmatrix} r_1 & 0 & \cdots & 0 \\ 0 & r_2 & \cdots & 0 \\ \vdots & 0 & \ddots & 0 \\ 0 & 0 & \cdots & r_n \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \cdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} = \begin{bmatrix} r_1 a_{11} & r_1 a_{12} & \cdots & r_1 a_{1n} \\ r_2 a_{21} & r_2 a_{22} & \cdots & r_2 a_{2n} \\ \vdots & \vdots & \cdots & \vdots \\ r_n a_{n1} & r_n a_{n2} & \cdots & r_n a_{nn} \end{bmatrix}$$

Numerical practice: $r_i \equiv 1 \Big/ \max\limits_{1 \le j \le n} \left| a_{ij} \right| \longrightarrow r_i = 2^m \approx 1 \Big/ \max\limits_{1 \le j \le n} \left| a_{ij} \right|$

Column Equilibration

$$c_j \equiv 1 \Big/ \max_{1\le i\le n} \left| a_{ij} \right| \qquad \left(1 \le j \le n\right)$$

$$\sum_{i=1}^{n} a_{ij} x_j = b_i \longrightarrow \sum_{i=1}^{n} \left(a_{ij} c_j\right) \left(\frac{x_j}{c_j}\right) = b_i$$

$$\mathbf{Ax} = \mathbf{b} \longrightarrow \left(\mathbf{AC}\right)\left(\mathbf{C}^{-1}\mathbf{x}\right) = \tilde{\mathbf{A}}\mathbf{z} = \mathbf{b}$$

$$\max_{1\le i\le n} \left| \tilde{a}_{ij} \right| = 1 \qquad \left(1 \le j \le n\right)$$

Right Multiplication

$$\mathbf{AC} = \tilde{\mathbf{A}}$$

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & \cdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} c_1 & 0 & \cdots & 0 \\ 0 & c_2 & \cdots & 0 \\ \vdots & 0 & \ddots & 0 \\ 0 & 0 & \cdots & c_n \end{bmatrix} = \begin{bmatrix} c_1 a_{11} & c_2 a_{12} & \cdots & c_n a_{1n} \\ c_1 a_{21} & c_2 a_{22} & \cdots & c_n a_{2n} \\ \vdots & \vdots & \cdots & \vdots \\ c_1 a_{n1} & c_2 a_{n2} & \cdots & c_n a_{nn} \end{bmatrix}$$

Numerical practice: $c_j \equiv 1 \Big/ \max\limits_{1 \le i \le n} \left| a_{ij} \right| \longrightarrow c_j = 2^m \approx 1 \Big/ \max\limits_{1 \le i \le n} \left| a_{ij} \right|$

Simple Scaling

$$\begin{cases} a_{11}x_1 + a_{12}x_2 + \ldots + a_{1n}x_n = b_1 & \times r_1 \\ a_{21}x_1 + a_{22}x_2 + \ldots + a_{2n}x_n = b_2 & \times r_2 \\ \vdots & \\ a_{n1}x_1 + a_{n2}x_2 + \ldots + a_{nn}x_n = b_n & \times r_n \end{cases}$$

Scaling + Pivoting = Scaled Pivoting

No Pivoting

- Diagonally dominant matrices
- Positive definite matrices

$$\left|a_{ii}\right| \geq \sum_{j \neq i} \left|a_{ij}\right| \qquad i = 1, \ldots, n$$

Gauss Elimination

GE = Elimination Procedure + Scaled Pivoting

1. Partial Pivoting
2. Full Pivoting
3. Variants of Scaling

$$\text{FLOPs(GE)} \sim 2/3n^3$$

Summary on GE

- Partial Pivoting
  - Equilibrate System of Equations
  - Pivoting by Columns
  - Simple Book-Keeping
    - Solution vector in original order
- Full Pivoting
  - Does not Require Equilibration
  - Pivoting by both Columns and Rows
  - More Complex Book-Keeping
    - Solution vector re-ordered

Bottom Lines on GE

- Scaled partial pivoting is almost as effective as full pivoting
- Partial pivoting is simplest and thus most common
- Neither method guarantees stability
- Scaled partial pivoting gives small residuals

James Hardy Wilkinson
1919-1986

- Forward error analysis gives too overestimated bounds
- Backward error analysis: the computed solution is the exact solution to a nearby problem
- GE with partial pivoting "gives exactly the right answer to nearly the right question."

Backward Error Analysis

$\mathbf{A}$ is $n \times n$ matrix $\qquad \mathbf{Ax} = \mathbf{b} \xrightarrow{GE} \tilde{\mathbf{x}} : \; \left(\mathbf{A} + \mathbf{E}\right)\tilde{\mathbf{x}} = \mathbf{b}$

$$\frac{\|\mathbf{E}\|_\infty}{\|\mathbf{A}\|_\infty} \le 1.01\left(n^3 + 3n^2\right) \cdot \rho \cdot \varepsilon_M \qquad \rho \equiv \frac{\max\limits_{1 \le i,j,k \le n} \left|a_{i,j}^{(k)}\right|}{\max\limits_{1 \le i,j \le n} \left|a_{i,j}\right|}$$

$$\frac{\|\mathbf{E}\|_\infty}{\|\mathbf{A}\|_\infty} \le n \cdot \varepsilon_M$$

Better empirical bound (Wilkinson)

$$\frac{\|\mathbf{E}\|_\infty}{\|\mathbf{A}\|_\infty} \le 2 \cdot \varepsilon_M$$

In most cases (Numerical practice)

Relative Residual

$$\mathbf{Ax} = \mathbf{b} \xrightarrow{GE} \tilde{\mathbf{x}} : \ \left(\mathbf{A} + \mathbf{E}\right)\tilde{\mathbf{x}} = \mathbf{b}$$

$$\left\|\mathbf{E}\right\|_\infty = \rho \cdot \beta^{-p} \cdot \left\|\mathbf{A}\right\|_\infty \qquad \rho \le \beta$$ Almost always

$$\mathbf{r} \equiv \mathbf{b} - \mathbf{A}\tilde{\mathbf{x}} = \mathbf{E}\tilde{\mathbf{x}} \longrightarrow \left\|\mathbf{b} - \mathbf{A}\tilde{\mathbf{x}}\right\| \le \left\|\mathbf{E}\right\| \cdot \left\|\tilde{\mathbf{x}}\right\|$$

$$\frac{\left\|\mathbf{b} - \mathbf{A}\tilde{\mathbf{x}}\right\|_\infty}{\left\|\mathbf{A}\right\|_\infty \cdot \left\|\tilde{\mathbf{x}}\right\|_\infty} \le \frac{\left\|\mathbf{E}\right\|_\infty}{\left\|\mathbf{A}\right\|_\infty} = \rho \cdot \beta^{-p} = \rho \cdot \varepsilon_M$$

Relative Error

$$\mathbf{x}-\tilde{\mathbf{x}}=\mathbf{A}^{-1}\left(\mathbf{b}-\mathbf{A}\tilde{\mathbf{x}}\right)\longrightarrow\left\|\mathbf{x}-\tilde{\mathbf{x}}\right\|\le\left\|\mathbf{A}^{-1}\right\|\cdot\left\|\mathbf{E}\right\|\cdot\left\|\tilde{\mathbf{x}}\right\|$$

$$\frac{\left\|\mathbf{x}-\tilde{\mathbf{x}}\right\|_\infty}{\left\|\tilde{\mathbf{x}}\right\|_\infty}\le\left\|\mathbf{A}^{-1}\right\|_\infty\cdot\left\|\mathbf{E}\right\|_\infty=\rho\beta^{-p}\left\|\mathbf{A}^{-1}\right\|_\infty\cdot\left\|\mathbf{A}\right\|_\infty=\kappa_\infty\left(\mathbf{A}\right)\cdot\rho\beta^{-p}$$

$$\frac{\left\|\mathbf{x}-\tilde{\mathbf{x}}\right\|_\infty}{\left\|\tilde{\mathbf{x}}\right\|_\infty}\le\varepsilon_{rel}\longrightarrow d=\log_{10}\frac{1}{\varepsilon_{rel}}\approx\log_{10}\left(\beta^{p-1}\right)-\log_{10}\kappa_\infty\left(\mathbf{A}\right)$$

Best Practice

- Investigate the condition number
  - Exact $\kappa(A)$ is tricky
  - In MATLAB, use `condest`
- Consistent with physics
  - E.g. don't couple domains that are physically uncoupled
- Consistent units
  - Don't mix meters and micro-meters
- Dimensionless unknowns
  - Normalise all unknowns consistently

Important

- Explicit Solutions
- Determinants
- Gauss Elimination
- LU Decomposition
- Pivoting
- Scaling
- Backward Error Analysis