Lecture Notes to Accompany

Scientific Computing

An Introductory Survey

Second Edition

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Chapter 2

Systems of Linear Equations

Systems of Linear Equations

Given $m \times n$ matrix $\boldsymbol{A}$ and m-vector $\boldsymbol{b}$, find unknown n-vector $\boldsymbol{x}$ satisfying

$$\boldsymbol{Ax} = \boldsymbol{b}$$

System of equations asks "Can $\boldsymbol{b}$ be expressed as linear combination of columns of $\boldsymbol{A}$?"

If so, coefficients of linear combination given by components of solution vector $\boldsymbol{x}$

Solution may or may not exist, and may or may not be unique

For now, we consider only *square* case, $m = n$

Singularity and Nonsingularity

$n \times n$ matrix $\boldsymbol{A}$ is *nonsingular* if it has any of following equivalent properties:

1. Inverse of $\boldsymbol{A}$, denoted by $\boldsymbol{A}^{-1}$, exists
2. $\det(\boldsymbol{A}) \neq 0$
3. $\operatorname{rank}(\boldsymbol{A}) = n$
4. For any vector $\boldsymbol{z} \neq \boldsymbol{o}$, $\boldsymbol{A}\boldsymbol{z} \neq \boldsymbol{o}$

Singularity and Nonsingularity, cont.

Solvability of $\boldsymbol{Ax} = \boldsymbol{b}$ depends on whether $\boldsymbol{A}$ is singular or nonsingular

If $\boldsymbol{A}$ is nonsingular, then $\boldsymbol{Ax} = \boldsymbol{b}$ has unique solution for any $\boldsymbol{b}$

If $\boldsymbol{A}$ is singular, then number of solutions is determined by $\boldsymbol{b}$

If $\boldsymbol{A}$ is singular and $\boldsymbol{Ax} = \boldsymbol{b}$, then $\boldsymbol{A}(\boldsymbol{x}+\gamma\boldsymbol{z}) = \boldsymbol{b}$ for any scalar γ, where $\boldsymbol{Az} = \boldsymbol{o}$ and $\boldsymbol{z} \neq \boldsymbol{o}$, so solution not unique

One solution:	nonsingular
No solution:	singular
∞ many solutions:	singular

Geometric Interpretation

In two dimensions, each equation determines straight line in plane

Intersection point of two lines is solution

If two straight lines not parallel (nonsingular), then intersection point unique

If two straight lines parallel (singular), then lines either do not intersect (no solution) or else coincide (any point along line is solution)

In higher dimensions, each equation determines hyperplane. If matrix nonsingular, intersection of hyperplanes is unique solution

Example: Nonsingularity

2×2 system

$$\begin{aligned} 2x_1 + 3x_2 &= b_1, \\ 5x_1 + 4x_2 &= b_2, \end{aligned}$$

or in matrix-vector notation

$$\boldsymbol{Ax} = \begin{bmatrix} 2 & 3 \\ 5 & 4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} = \boldsymbol{b},$$

is nonsingular regardless of value of $\boldsymbol{b}$

For example, if $\boldsymbol{b} = [\,8 \quad 13\,]^T$, then $\boldsymbol{x} = [\,1 \quad 2\,]^T$ is unique solution

Example: Singularity

2×2 system

$$\boldsymbol{Ax} = \begin{bmatrix} 2 & 3 \\ 4 & 6 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix} = \boldsymbol{b}$$

is singular regardless of value of $\boldsymbol{b}$

With $\boldsymbol{b} = [\,4 \quad 7\,]^T$, there is no solution

With $\boldsymbol{b} = [\,4 \quad 8\,]^T$, $\boldsymbol{x} = [\,\gamma \quad (4 - 2\gamma)/3\,]^T$ is solution for any real number γ

Vector Norms

Magnitude, modulus, or absolute value for scalars generalizes to *norm* for vectors

We will use only p-norms, defined by

$$\|\boldsymbol{x}\|_p = \left(\sum_{i=1}^{n} |x_i|^p \right)^{1/p}$$

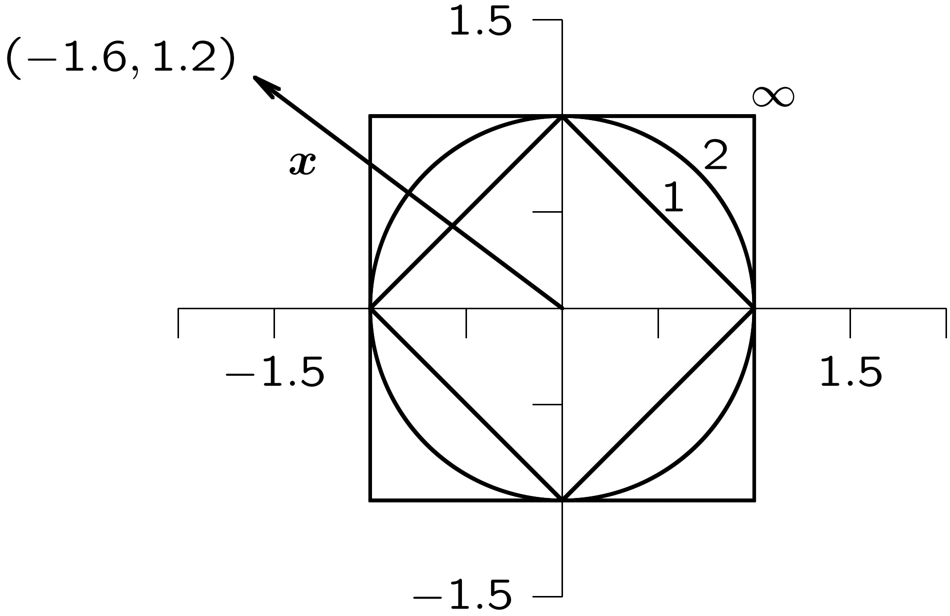
for integer $p > 0$ and n-vector $\boldsymbol{x}$

Important special cases:

- 1-norm: $\|\boldsymbol{x}\|_1 = \sum_{i=1}^{n} |x_i|$
- 2-norm: $\|\boldsymbol{x}\|_2 = \left(\sum_{i=1}^{n} |x_i|^2 \right)^{1/2}$
- ∞-norm: $\|\boldsymbol{x}\|_\infty = \max_i |x_i|$

Vector Norms, continued

Drawing shows unit sphere in two dimensions for each of these norms:



Norms have following values for vector shown:

$$\|\boldsymbol{x}\|_1 = 2.8, \quad \|\boldsymbol{x}\|_2 = 2.0, \quad \|\boldsymbol{x}\|_\infty = 1.6$$

In general, for any vector $\boldsymbol{x}$ in $\mathbb{R}^n$,

$$\|\boldsymbol{x}\|_1 \geq \|\boldsymbol{x}\|_2 \geq \|\boldsymbol{x}\|_\infty$$

Properties of Vector Norms

For any vector norm,

1. $\|\boldsymbol{x}\| > 0$ if $\boldsymbol{x} \neq \boldsymbol{o}$

2. $\|\gamma\boldsymbol{x}\| = |\gamma| \cdot \|\boldsymbol{x}\|$ for any scalar γ

3. $\|\boldsymbol{x}+\boldsymbol{y}\| \leq \|\boldsymbol{x}\|+\|\boldsymbol{y}\|$ (triangle inequality)

In more general treatment, these properties taken as *definition* of vector norm

Useful variation on triangle inequality:

$$|\,\|\boldsymbol{x}\| - \|\boldsymbol{y}\|\,| \leq \|\boldsymbol{x} - \boldsymbol{y}\|$$

Matrix Norms

Matrix norm corresponding to given vector norm defined by

$$\|\boldsymbol{A}\| = \max_{\boldsymbol{x} \neq \boldsymbol{o}} \frac{\|\boldsymbol{A}\boldsymbol{x}\|}{\|\boldsymbol{x}\|}$$

Norm of matrix measures maximum stretching matrix does to any vector in given vector norm

Matrix norm corresponding to vector 1-norm is maximum absolute column sum,

$$\|\boldsymbol{A}\|_1 = \max_j \sum_{i=1}^{n} |a_{ij}|$$

Matrix norm corresponding to vector ∞-norm is maximum absolute row sum,

$$\|\boldsymbol{A}\|_\infty = \max_i \sum_{j=1}^{n} |a_{ij}|$$

Properties of Matrix Norms

Any matrix norm satisfies:

1. $\|\boldsymbol{A}\| > 0$ if $\boldsymbol{A} \neq \boldsymbol{O}$

2. $\|\gamma \boldsymbol{A}\| = |\gamma| \cdot \|\boldsymbol{A}\|$ for any scalar γ

3. $\|\boldsymbol{A} + \boldsymbol{B}\| \leq \|\boldsymbol{A}\| + \|\boldsymbol{B}\|$

Matrix norms we have defined also satisfy

4. $\|\boldsymbol{AB}\| \leq \|\boldsymbol{A}\| \cdot \|\boldsymbol{B}\|$

5. $\|\boldsymbol{Ax}\| \leq \|\boldsymbol{A}\| \cdot \|\boldsymbol{x}\|$ for any vector $\boldsymbol{x}$

Condition Number of Matrix

Condition number of square nonsingular matrix $\boldsymbol{A}$ defined by

$$\text{cond}(\boldsymbol{A}) = \|\boldsymbol{A}\| \cdot \|\boldsymbol{A}^{-1}\|$$

By convention, $\text{cond}(\boldsymbol{A}) = \infty$ if $\boldsymbol{A}$ singular

Since

$$\|\boldsymbol{A}\| \cdot \|\boldsymbol{A}^{-1}\| = \left(\max_{\boldsymbol{x} \neq \boldsymbol{o}} \frac{\|\boldsymbol{A}\boldsymbol{x}\|}{\|\boldsymbol{x}\|} \right) \cdot \left(\min_{\boldsymbol{x} \neq \boldsymbol{o}} \frac{\|\boldsymbol{A}\boldsymbol{x}\|}{\|\boldsymbol{x}\|} \right)^{-1},$$

condition number measures ratio of maximum stretching to maximum shrinking matrix does to any nonzero vectors

Large $\text{cond}(\boldsymbol{A})$ means $\boldsymbol{A}$ nearly singular

Properties of Condition Number

1. For any matrix $\boldsymbol{A}$, cond$(\boldsymbol{A}) \geq 1$

2. For identity matrix, cond$(\boldsymbol{I}) = 1$

3. For any matrix $\boldsymbol{A}$ and scalar γ,

$$\text{cond}(\gamma \boldsymbol{A}) = \text{cond}(\boldsymbol{A})$$

4. For any diagonal matrix $\boldsymbol{D} = \text{diag}(d_i)$,

$$\text{cond}(\boldsymbol{D}) = (\max |d_i|)/(\min |d_i|)$$

Computing Condition Number

Definition of condition number involves matrix inverse, so nontrivial to compute

Computing condition number from definition would require much more work than computing solution whose accuracy to be assessed

In practice, condition number estimated inexpensively as byproduct of solution process

Matrix norm $\|\boldsymbol{A}\|$ easily computed as maximum absolute column sum (or row sum, depending on norm used)

Estimating $\|\boldsymbol{A}^{-1}\|$ at low cost more challenging

Computing Condition Number, cont.

From properties of norms, if $\boldsymbol{A}\boldsymbol{z} = \boldsymbol{y}$, then

$$\frac{\|\boldsymbol{z}\|}{\|\boldsymbol{y}\|} \leq \|\boldsymbol{A}^{-1}\|,$$

and bound achieved for optimally chosen $\boldsymbol{y}$

Efficient condition estimators heuristically pick $\boldsymbol{y}$ with large ratio $\|\boldsymbol{z}\|/\|\boldsymbol{y}\|$, yielding good estimate for $\|\boldsymbol{A}^{-1}\|$

Good software packages for linear systems provide efficient and reliable condition estimator

Error Bounds

Condition number yields error bound for computed solution to linear system

Let $\boldsymbol{x}$ be solution to $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$, and let $\hat{\boldsymbol{x}}$ be solution to $\boldsymbol{A}\hat{\boldsymbol{x}} = \boldsymbol{b} + \Delta\boldsymbol{b}$

If $\Delta\boldsymbol{x} = \hat{\boldsymbol{x}} - \boldsymbol{x}$, then

$$\boldsymbol{b} + \Delta\boldsymbol{b} = \boldsymbol{A}(\hat{\boldsymbol{x}}) = \boldsymbol{A}(\boldsymbol{x} + \Delta\boldsymbol{x}) = \boldsymbol{A}\boldsymbol{x} + \boldsymbol{A}\Delta\boldsymbol{x},$$

which leads to bound

$$\frac{\|\Delta\boldsymbol{x}\|}{\|\boldsymbol{x}\|} \leq \mathrm{cond}(\boldsymbol{A})\frac{\|\Delta\boldsymbol{b}\|}{\|\boldsymbol{b}\|}$$

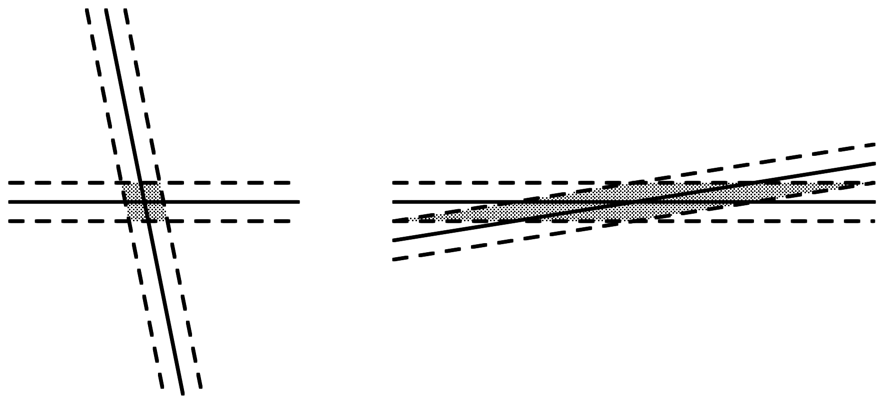
for possible relative change in solution due to relative change in right-hand side $\boldsymbol{b}$

Error Bounds, continued

Similar result holds for relative change in matrix: if $(\boldsymbol{A}+\boldsymbol{E})\hat{\boldsymbol{x}} = \boldsymbol{b}$, then

$$\frac{\|\Delta \boldsymbol{x}\|}{\|\hat{\boldsymbol{x}}\|} \leq \text{cond}(\boldsymbol{A}) \frac{\|\boldsymbol{E}\|}{\|\boldsymbol{A}\|}$$

In two dimensions, uncertainty in intersection point of two lines depends on whether lines nearly parallel



well-conditioned　　　ill-conditioned

Error Bounds, continued

If input data accurate to machine precision, then bound for relative error in computed solution given by

$$\frac{\|\hat{\boldsymbol{x}} - \boldsymbol{x}\|}{\|\boldsymbol{x}\|} \leq \text{cond}(\boldsymbol{A})\, \epsilon_{\text{mach}}$$

Computed solution loses about $\log_{10}(\text{cond}(\boldsymbol{A}))$ decimal digits accuracy relative to accuracy of input

We will later see example using 3-digit precision for problem with cond $> 10^3$, which yields no correct digits in solution

Caveats

1. Normwise analysis bounds relative error in *largest* components of solution; relative error in smaller components can be much larger

Componentwise error bounds can be obtained, but somewhat more complicated

2. Conditioning of system affected by scaling

Ill-conditioning can result from poor scaling as well as near singularity

Rescaling can help former, but not latter

Residual

Residual vector of approximate solution $\hat{\boldsymbol{x}}$ to linear system $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$ defined by

$$\boldsymbol{r} = \boldsymbol{b} - \boldsymbol{A}\hat{\boldsymbol{x}}$$

In theory, if $\boldsymbol{A}$ is nonsingular, then $\|\hat{\boldsymbol{x}} - \boldsymbol{x}\| = 0$ if, and only if, $\|\boldsymbol{r}\| = 0$, but they are not necessarily small simultaneously

Since

$$\frac{\|\Delta \boldsymbol{x}\|}{\|\hat{\boldsymbol{x}}\|} \le \text{cond}(\boldsymbol{A}) \frac{\|\boldsymbol{r}\|}{\|\boldsymbol{A}\| \cdot \|\hat{\boldsymbol{x}}\|},$$

small relative residual implies small relative error only if $\boldsymbol{A}$ well-conditioned

Residual, continued

If computed solution $\hat{\boldsymbol{x}}$ exactly satisfies

$$(\boldsymbol{A} + \boldsymbol{E})\hat{\boldsymbol{x}} = \boldsymbol{b},$$

then

$$\frac{\|\boldsymbol{r}\|}{\|\boldsymbol{A}\| \; \|\hat{\boldsymbol{x}}\|} \leq \frac{\|\boldsymbol{E}\|}{\|\boldsymbol{A}\|},$$

so large *relative residual* implies large backward error in matrix, and algorithm used to compute solution is unstable

Stable algorithm yields small relative residual regardless how ill-conditioned nonsingular system may be

Solving Linear Systems

To solve linear system, transform it into one whose solution is same but easier to compute

What type of transformation of linear system leaves solution unchanged?

We can premultiply (from left) both sides of linear system $\boldsymbol{Ax} = \boldsymbol{b}$ by any nonsingular matrix $\boldsymbol{M}$ without affecting solution

Solution to $\boldsymbol{MAx} = \boldsymbol{Mb}$ is given by

$$\boldsymbol{x} = (\boldsymbol{MA})^{-1}\boldsymbol{Mb} = \boldsymbol{A}^{-1}\boldsymbol{M}^{-1}\boldsymbol{Mb} = \boldsymbol{A}^{-1}\boldsymbol{b}$$

Example: Permutations

Permutation matrix $\boldsymbol{P}$ has one 1 in each row and column and zeros elsewhere. $\boldsymbol{P}^{-1} = \boldsymbol{P}^T$

Premultiplying both sides of system by permutation matrix, $\boldsymbol{PAx} = \boldsymbol{Pb}$, reorders rows, but solution $\boldsymbol{x}$ unchanged

Postmultiplying $\boldsymbol{A}$ by permutation matrix, $\boldsymbol{APx} = \boldsymbol{b}$, reorders columns, which permutes components of original solution:

$$\boldsymbol{x} = (\boldsymbol{AP})^{-1}\boldsymbol{b} = \boldsymbol{P}^{-1}\boldsymbol{A}^{-1}\boldsymbol{b} = \boldsymbol{P}^T(\boldsymbol{A}^{-1}\boldsymbol{b})$$

Example: Diagonal Scaling

Row scaling: Premultiplying both sides of system by nonsingular diagonal matrix $\boldsymbol{D}$, $\boldsymbol{DAx} = \boldsymbol{Db}$, multiplies each row of matrix and right-hand side by corresponding diagonal entry of $\boldsymbol{D}$, but solution $\boldsymbol{x}$ unchanged

Column scaling: postmultiplying $\boldsymbol{A}$ by $\boldsymbol{D}$, $\boldsymbol{ADx} = \boldsymbol{b}$, multiplies each column of matrix by corresponding diagonal entry of $\boldsymbol{D}$, which rescales original solution:

$$\boldsymbol{x} = (\boldsymbol{AD})^{-1}\boldsymbol{b} = \boldsymbol{D}^{-1}\boldsymbol{A}^{-1}\boldsymbol{b}$$

Triangular Linear Systems

Next question is, what type of linear system is easy to solve?

If one equation in system involves only one component of solution (i.e., only one entry in that row of matrix is nonzero), then that component can be computed by division

If another equation in system involves only one additional solution component, then by substituting one known component into it, we can solve for other component

If this pattern continues, with only one new solution component per equation, then all components of solution can be computed in succession.

System with this property called *triangular*

Triangular Matrices

Matrix is *lower triangular* if all entries above main diagonal are zero: $a_{ij} = 0$ for $i < j$

Matrix is *upper triangular* if all entries below main diagonal are zero: $a_{ij} = 0$ for $i > j$

Any triangular matrix can be permuted into upper or lower triangular form by suitable row permutation

Forward- and Back-Substitution

Forward-substitution for lower triangular system $\boldsymbol{L}\boldsymbol{x} = \boldsymbol{b}$:

$$x_1 = b_1/\ell_{11},$$

$$x_i = \left(b_i - \sum_{j=1}^{i-1} \ell_{ij} x_j \right) / \ell_{ii}, \quad i = 2, \ldots, n$$

Back-substitution for upper triangular system $\boldsymbol{U}\boldsymbol{x} = \boldsymbol{b}$:

$$x_n = b_n/u_{nn},$$

$$x_i = \left(b_i - \sum_{j=i+1}^{n} u_{ij} x_j \right) / u_{ii}, \quad i = n-1, \ldots, 1$$

Example: Triangular Linear System

$$\begin{bmatrix} 2 & 4 & -2 \\ 0 & 1 & 1 \\ 0 & 0 & 4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 2 \\ 4 \\ 8 \end{bmatrix}$$

Last equation, $4x_3 = 8$, can be solved directly to obtain $x_3 = 2$

x_3 then substituted into second equation to obtain $x_2 = 2$

Finally, both x_3 and x_2 substituted into first equation to obtain $x_1 = -1$

Elimination

To transform general linear system into triangular form, need to replace selected nonzero entries of matrix by zeros

This can be accomplished by taking linear combinations of rows

Consider 2-vector $\boldsymbol{a} = \begin{bmatrix} a_1 \\ a_2 \end{bmatrix}$

If $a_1 \neq 0$, then

$$\begin{bmatrix} 1 & 0 \\ -a_2/a_1 & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \end{bmatrix} = \begin{bmatrix} a_1 \\ 0 \end{bmatrix}$$

Elementary Elimination Matrices

More generally, can annihilate *all* entries below kth position in n-vector $\boldsymbol{a}$ by transformation $\boldsymbol{M}_k\boldsymbol{a} =$

$$\begin{bmatrix} 1 & \cdots & 0 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 1 & 0 & \cdots & 0 \\ 0 & \cdots & -m_{k+1} & 1 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & -m_n & 0 & \cdots & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ \vdots \\ a_k \\ a_{k+1} \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} a_1 \\ \vdots \\ a_k \\ 0 \\ \vdots \\ 0 \end{bmatrix},$$

where $m_i = a_i/a_k$, $i = k+1, \ldots, n$

Divisor a_k, called *pivot*, must be nonzero

Matrix $\boldsymbol{M}_k$, called *elementary elimination* matrix, adds multiple of row k to each subsequent row, with multipliers m_i chosen so that result is zero

Elementary Elimination Matrices, cont.

$\boldsymbol{M}_k$ is unit lower triangular and nonsingular

$\boldsymbol{M}_k = \boldsymbol{I} - \boldsymbol{m}_k \boldsymbol{e}_k^T$, where

$$\boldsymbol{m}_k = [0, \ldots, 0, m_{k+1}, \ldots, m_n]^T$$

and $\boldsymbol{e}_k$ is kth column of identity matrix

$\boldsymbol{M}_k^{-1} = \boldsymbol{I} + \boldsymbol{m}_k \boldsymbol{e}_k^T$, which means $\boldsymbol{M}_k^{-1} = \boldsymbol{L}_k$ same as $\boldsymbol{M}_k$ except signs of multipliers reversed

If $\boldsymbol{M}_j$, $j > k$, is another elementary elimination matrix, with vector of multipliers $\boldsymbol{m}_j$, then

$$\begin{aligned} \boldsymbol{M}_k \boldsymbol{M}_j &= \boldsymbol{I} - \boldsymbol{m}_k \boldsymbol{e}_k^T - \boldsymbol{m}_j \boldsymbol{e}_j^T + \boldsymbol{m}_k \boldsymbol{e}_k^T \boldsymbol{m}_j \boldsymbol{e}_j^T \\ &= \boldsymbol{I} - \boldsymbol{m}_k \boldsymbol{e}_k^T - \boldsymbol{m}_j \boldsymbol{e}_j^T, \end{aligned}$$

which means product is essentially "union," and similarly for product of inverses, $\boldsymbol{L}_k \boldsymbol{L}_j$

Example: Elementary Elim. Matrices

If $\boldsymbol{a} = \begin{bmatrix} 2 \\ 4 \\ -2 \end{bmatrix}$, then

$$\boldsymbol{M}_1\boldsymbol{a} = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 4 \\ -2 \end{bmatrix} = \begin{bmatrix} 2 \\ 0 \\ 0 \end{bmatrix}$$

$$\boldsymbol{M}_2\boldsymbol{a} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1/2 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 4 \\ -2 \end{bmatrix} = \begin{bmatrix} 2 \\ 4 \\ 0 \end{bmatrix}$$

Note that

$$\boldsymbol{L}_1 = \boldsymbol{M}_1^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -1 & 0 & 1 \end{bmatrix}$$

$$\boldsymbol{L}_2 = \boldsymbol{M}_2^{-1} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1/2 & 1 \end{bmatrix}$$

Example Continued

Further note that

$$M_1 M_2 = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 1 & 1/2 & 1 \end{bmatrix}$$

$$L_1 L_2 = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -1 & -1/2 & 1 \end{bmatrix}$$

Gaussian Elimination

To reduce general linear system $\boldsymbol{Ax} = \boldsymbol{b}$ to upper triangular form, first choose $\boldsymbol{M}_1$, with a_{11} as pivot, to annihilate first column of $\boldsymbol{A}$ below first row

System becomes $\boldsymbol{M}_1\boldsymbol{Ax} = \boldsymbol{M}_1\boldsymbol{b}$, but solution unchanged

Next choose $\boldsymbol{M}_2$, using a_{22} as pivot, to annihilate second column of $\boldsymbol{M}_1\boldsymbol{A}$ below second row. System becomes $\boldsymbol{M}_2\boldsymbol{M}_1\boldsymbol{Ax} = \boldsymbol{M}_2\boldsymbol{M}_1\boldsymbol{b}$, but solution still unchanged

Process continues for each successive column until all subdiagonal entries have been zeroed

Resulting upper triangular linear system

$$\boldsymbol{MAx} = \boldsymbol{M}_{n-1}\cdots\boldsymbol{M}_1\boldsymbol{Ax} = \boldsymbol{M}_{n-1}\cdots\boldsymbol{M}_1\boldsymbol{b} = \boldsymbol{Mb}$$

can be solved by back-substitution to obtain solution to original linear system $\boldsymbol{Ax} = \boldsymbol{b}$

LU Factorization

Product $\boldsymbol{L}_k \boldsymbol{L}_j$ unit lower triangular if $k < j$, so

$$\boldsymbol{L} = \boldsymbol{M}^{-1} = \boldsymbol{M}_1^{-1} \cdots \boldsymbol{M}_{n-1}^{-1} = \boldsymbol{L}_1 \cdots \boldsymbol{L}_{n-1}$$

unit lower triangular

By design, $\boldsymbol{U} = \boldsymbol{M}\boldsymbol{A}$ upper triangular

So $\boldsymbol{A} = \boldsymbol{L}\boldsymbol{U}$, with $\boldsymbol{L}$ unit lower triangular and $\boldsymbol{U}$ upper triangular

Thus, $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$ becomes $\boldsymbol{L}\boldsymbol{U}\boldsymbol{x} = \boldsymbol{b}$, and can be solved by forward-substitution in lower triangular system $\boldsymbol{L}\boldsymbol{y} = \boldsymbol{b}$, followed by back-substitution in upper triangular system $\boldsymbol{U}\boldsymbol{x} = \boldsymbol{y}$

$\boldsymbol{y} = \boldsymbol{M}\boldsymbol{b}$, transformed right hand side in Gaussian elimination

Gaussian elimination and LU factorization are two ways of expressing same solution process

Example: Gaussian Elimination

Use Gaussian elimination to solve linear system

$$\begin{bmatrix} 2 & 4 & -2 \\ 4 & 9 & -3 \\ -2 & -3 & 7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 2 \\ 8 \\ 10 \end{bmatrix}$$

To annihilate subdiagonal entries of first column of $\boldsymbol{A}$, $\boldsymbol{M}_1\boldsymbol{A} =$

$$\begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2 & 4 & -2 \\ 4 & 9 & -3 \\ -2 & -3 & 7 \end{bmatrix} = \begin{bmatrix} 2 & 4 & -2 \\ 0 & 1 & 1 \\ 0 & 1 & 5 \end{bmatrix}$$

$$\boldsymbol{M}_1\boldsymbol{b} = \begin{bmatrix} 1 & 0 & 0 \\ -2 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 8 \\ 10 \end{bmatrix} = \begin{bmatrix} 2 \\ 4 \\ 12 \end{bmatrix}$$

Example Continued

To annihilate subdiagonal entry of second column of $\boldsymbol{M}_1\boldsymbol{A}$, $\boldsymbol{M}_2\boldsymbol{M}_1\boldsymbol{A} =$

$$\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} 2 & 4 & -2 \\ 0 & 1 & 1 \\ 0 & 1 & 5 \end{bmatrix} = \begin{bmatrix} 2 & 4 & -2 \\ 0 & 1 & 1 \\ 0 & 0 & 4 \end{bmatrix}$$

$$\boldsymbol{M}_2\boldsymbol{M}_1\boldsymbol{b} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} 2 \\ 4 \\ 12 \end{bmatrix} = \begin{bmatrix} 2 \\ 4 \\ 8 \end{bmatrix}$$

We have reduced original system to equivalent upper triangular system

$$\begin{bmatrix} 2 & 4 & -2 \\ 0 & 1 & 1 \\ 0 & 0 & 4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 2 \\ 4 \\ 8 \end{bmatrix}$$

which can now be solved by back-substitution to obtain $\boldsymbol{x} = [\,-1 \quad 2 \quad 2\,]^T$

Example Continued

To write out LU factorization explicitly,
$\boldsymbol{L} = \boldsymbol{L}_1 \boldsymbol{L}_2 =$

$$\begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -1 & 1 & 1 \end{bmatrix}$$

so that

$$\begin{bmatrix} 2 & 4 & -2 \\ 4 & 9 & -3 \\ -2 & -3 & 7 \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ -1 & 1 & 1 \end{bmatrix} \begin{bmatrix} 2 & 4 & -2 \\ 0 & 1 & 1 \\ 0 & 0 & 4 \end{bmatrix}$$

Row Interchanges

Gaussian elimination breaks down if leading diagonal entry of remaining unreduced matrix is zero at any stage

Solution easy: if diagonal entry is zero at stage k, then interchange row k with some subsequent row having nonzero entry in column k and proceed as usual

What if there is no nonzero on or below diagonal in column k?

Then nothing to do at this stage, so move on to next column

This leaves zero on diagonal, so resulting upper triangular matrix $\boldsymbol{U}$ singular, but LU factorization can still be completed

Subsequent back-substitution will fail, however, as it should for singular matrix

Partial Pivoting

In principle, any nonzero value will do as pivot, but in practice choice should be made to minimize error

Should avoid amplifying previous rounding errors when multiplying remaining portion of matrix by elementary elimination matrix

So multipliers should not exceed 1 in magnitude, which can be accomplished by choosing entry of largest magnitude on or below diagonal as pivot

Such *partial pivoting* is essential in practice for numerically stable implementation of Gaussian elimination for general linear systems

LU with Partial Pivoting

With partial pivoting, each $\boldsymbol{M}_k$ preceded by $\boldsymbol{P}_k$, permutation interchanging rows to bring entry of largest magnitude into diagonal pivot position

Still have $\boldsymbol{MA} = \boldsymbol{U}$, with $\boldsymbol{U}$ upper triangular, but now

$$\boldsymbol{M} = \boldsymbol{M}_{n-1}\boldsymbol{P}_{n-1}\cdots\boldsymbol{M}_1\boldsymbol{P}_1$$

$\boldsymbol{M}^{-1}$ still triangular in general sense, but because of permutations, $\boldsymbol{M}^{-1}$ not necessarily *lower* triangular, but still denoted by $\boldsymbol{L}$

Alternatively, can write

$$\boldsymbol{PA} = \boldsymbol{LU},$$

where $\boldsymbol{P} = \boldsymbol{P}_{n-1}\cdots\boldsymbol{P}_1$ permutes rows of $\boldsymbol{A}$ into order determined by partial pivoting, and now $\boldsymbol{L}$ really is lower triangular

Complete Pivoting

Complete pivoting is more exhaustive strategy where largest entry in entire remaining unreduced submatrix is permuted into diagonal pivot position

Requires interchanging columns as well as rows, leading to factorization

$$\boldsymbol{PAQ} = \boldsymbol{LU},$$

with $\boldsymbol{L}$ unit lower triangular, $\boldsymbol{U}$ upper triangular, and $\boldsymbol{P}$ and $\boldsymbol{Q}$ permutations

Numerical stability of complete pivoting theoretically superior, but pivot search more expensive than partial pivoting

Numerical stability of partial pivoting more than adequate in practice, so almost always used in solving linear systems by Gaussian elimination

Example: Pivoting

Need for pivoting has nothing to do with whether matrix is singular or nearly singular

For example,

$$\boldsymbol{A} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

is nonsingular yet has no LU factorization unless rows interchanged, whereas

$$\boldsymbol{A} = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$$

is singular yet has LU factorization

Example: Small Pivots

To illustrate effect of small pivots, consider

$$\boldsymbol{A} = \begin{bmatrix} \epsilon & 1 \\ 1 & 1 \end{bmatrix},$$

where ϵ is positive number smaller than ϵ_{mach}

If rows not interchanged, then pivot is ϵ and multiplier is $-1/\epsilon$, so

$$\boldsymbol{M} = \begin{bmatrix} 1 & 0 \\ -1/\epsilon & 1 \end{bmatrix}, \quad \boldsymbol{L} = \begin{bmatrix} 1 & 0 \\ 1/\epsilon & 1 \end{bmatrix},$$

$$\boldsymbol{U} = \begin{bmatrix} \epsilon & 1 \\ 0 & 1 - 1/\epsilon \end{bmatrix} = \begin{bmatrix} \epsilon & 1 \\ 0 & -1/\epsilon \end{bmatrix}$$

in floating-point arithmetic. But then

$$\boldsymbol{LU} = \begin{bmatrix} 1 & 0 \\ 1/\epsilon & 1 \end{bmatrix} \begin{bmatrix} \epsilon & 1 \\ 0 & -1/\epsilon \end{bmatrix} = \begin{bmatrix} \epsilon & 1 \\ 1 & 0 \end{bmatrix} \neq \boldsymbol{A}$$

Example Continued

Using small pivot, and correspondingly large multiplier, has caused unrecoverable loss of information in transformed matrix

If rows interchanged, then pivot is 1 and multiplier is $-\epsilon$, so

$$\boldsymbol{M} = \begin{bmatrix} 1 & 0 \\ -\epsilon & 1 \end{bmatrix}, \quad \boldsymbol{L} = \begin{bmatrix} 1 & 0 \\ \epsilon & 1 \end{bmatrix},$$

$$\boldsymbol{U} = \begin{bmatrix} 1 & 1 \\ 0 & 1-\epsilon \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}$$

in floating-point arithmetic

Thus,

$$\boldsymbol{LU} = \begin{bmatrix} 1 & 0 \\ \epsilon & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ \epsilon & 1 \end{bmatrix},$$

which is correct after permutation

Pivoting, continued

Although pivoting generally required for stability of Gaussian elimination, pivoting *not* required for some important classes of matrices:

- *Diagonally dominant*:

$$\sum_{i=1,\, i\neq j}^{n} |a_{ij}| < |a_{jj}|, \quad j = 1, \ldots, n$$

- *Symmetric positive definite*:

$$\boldsymbol{A} = \boldsymbol{A}^T \quad \text{and} \quad \boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x} > 0 \text{ for all } \boldsymbol{x} \neq \boldsymbol{o}$$

Residual

Recall that residual $\boldsymbol{r} = \boldsymbol{b} - \boldsymbol{A}\hat{\boldsymbol{x}}$ satisfies

$$\frac{\|\boldsymbol{r}\|}{\|\boldsymbol{A}\| \ \|\hat{\boldsymbol{x}}\|} \leq \frac{\|\boldsymbol{E}\|}{\|\boldsymbol{A}\|},$$

where $\boldsymbol{E}$ is backward error in matrix $\boldsymbol{A}$

How large is $\|\boldsymbol{E}\|$ likely to be in practice?

For LU factorization by Gaussian elimination,

$$\frac{\|\boldsymbol{E}\|}{\|\boldsymbol{A}\|} \leq \rho \, n \, \epsilon_{\text{mach}},$$

where *growth factor* ρ is ratio of largest entry of $\boldsymbol{U}$ to largest entry of $\boldsymbol{A}$

Without pivoting, ρ can be arbitrarily large, so Gaussian elimination without pivoting is unstable

With partial pivoting, ρ can still be as large as 2^{n-1}, but such behavior extremely rare

Residual, continued

There is little or no growth in practice, so

$$\frac{\|\boldsymbol{E}\|}{\|\boldsymbol{A}\|} \approx n \, \epsilon_{\text{mach}},$$

which means Gaussian elimination with partial pivoting yields small relative residual regardless how ill-conditioned system is

Thus, small relative residual does not necessarily imply computed solution close to "true" solution unless system is well-conditioned

Complete pivoting yields even smaller growth factor, but additional margin of stability usually not worth extra cost

Example: Small Residual

Using 3-digit decimal arithmetic to solve

$$\begin{bmatrix} 0.641 & 0.242 \\ 0.321 & 0.121 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0.883 \\ 0.442 \end{bmatrix},$$

Gaussian elimination with partial pivoting yields triangular system

$$\begin{bmatrix} 0.641 & 0.242 \\ 0 & 0.000242 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0.883 \\ -0.000383 \end{bmatrix},$$

and back-substitution then gives solution

$$\boldsymbol{x} = [\,0.782 \quad 1.58\,]^T$$

Exact residual for this solution is

$$\boldsymbol{r} = \boldsymbol{b} - \boldsymbol{A}\boldsymbol{x} = \begin{bmatrix} -0.000622 \\ -0.000202 \end{bmatrix},$$

which is as small as can expect using 3-digit arithmetic

Example Continued

But exact solution is

$$\boldsymbol{x} = \begin{bmatrix} 1.00 \\ 1.00 \end{bmatrix},$$

so error is almost as large as solution

Cause of this phenomenon is that matrix is nearly singular (cond > 4000)

Division that determines x_2 is between two quantities that are both on order of rounding error, and hence result is essentially arbitrary

When arbitrary value for x_2 is substituted into first equation, value for x_1 is computed so that first equation is satisfied, yielding small residual, but poor solution

Implementation of Gaussian Elimination

Gaussian elimination, or LU factorization, has general form of triple-nested loop

```
for ______
    for ______
        for ______
            a_ij = a_ij - (a_ik/a_kk) a_kj
        end
    end
end
```

Indices i, j, and k of **for** loops can be taken in any order, for total of $3! = 6$ different ways of arranging loops

These variations have different memory access patterns, which may cause their performance to vary widely, depending on architectural features such as cache, paging, etc.

Uniqueness of LU Factorization

Despite variations in computing it, LU factorization unique up to diagonal scaling of factors

Provided row pivot sequence is same, if we have two LU factorizations $\boldsymbol{PA} = \boldsymbol{LU} = \hat{\boldsymbol{L}}\hat{\boldsymbol{U}}$, then $\hat{\boldsymbol{L}}^{-1}\boldsymbol{L} = \hat{\boldsymbol{U}}\boldsymbol{U}^{-1} = \boldsymbol{D}$ is both lower and upper triangular, hence diagonal

If both $\boldsymbol{L}$ and $\hat{\boldsymbol{L}}$ unit lower triangular, then $\boldsymbol{D}$ must be identity matrix, so $\boldsymbol{L} = \hat{\boldsymbol{L}}$ and $\boldsymbol{U} = \hat{\boldsymbol{U}}$

Uniqueness made explicit in LDU factorization $\boldsymbol{PA} = \boldsymbol{LDU}$, with $\boldsymbol{L}$ unit lower triangular, $\boldsymbol{U}$ unit upper triangular, and $\boldsymbol{D}$ diagonal

Storage Management

Elementary elimination matrices $\boldsymbol{M}_k$, their inverses $\boldsymbol{L}_k$, and permutation matrices $\boldsymbol{P}_k$ used in formal description of factorization process are *not* formed explicitly in actual implementation

$\boldsymbol{U}$ overwrites upper triangle of $\boldsymbol{A}$, multipliers in $\boldsymbol{L}$ overwrite strict lower triangle of $\boldsymbol{A}$, and unit diagonal of $\boldsymbol{L}$ need not be stored

Row interchanges usually not done explicitly; auxiliary integer vector keeps track of row order in original locations

Complexity of Solving Linear Systems

LU factorization requires about $n^3/3$ floating-point multiplications and similar number of additions

Forward- and back-substitution for single right-hand-side vector together require about n^2 multiplications and similar number of additions

Can also solve linear system by matrix inversion: $\boldsymbol{x} = \boldsymbol{A}^{-1}\boldsymbol{b}$

Computing $\boldsymbol{A}^{-1}$ tantamount to solving n linear systems, requiring LU factorization of $\boldsymbol{A}$ followed by n forward- and back-substitutions, one for each column of identity matrix

Operation count for inversion is about n^3, three times as expensive as LU factorization

Inversion vs Factorization

Even with many right-hand sides $\boldsymbol{b}$, inversion never overcomes higher initial cost, since each matrix-vector multiplication $\boldsymbol{A}^{-1}\boldsymbol{b}$ requires n^2 operations, similar to cost of forward- and back-substitution

Inversion gives less accurate answer. Simple example: solving system $3x = 18$ by division gives $x = 18/3 = 6$, but inversion gives $x = 3^{-1} \times 18 = 0.333 \times 18 = 5.99$ using 3-digit arithmetic

Matrix inverses often occur as convenient notation in formulas, but explicit inverse rarely required to implement such formulas

For example, product $\boldsymbol{A}^{-1}\boldsymbol{B}$ should be computed by LU factorization of $\boldsymbol{A}$, followed by forward- and back-substitutions using each column of $\boldsymbol{B}$

Gauss-Jordan Elimination

In Gauss-Jordan elimination, matrix reduced to diagonal rather than triangular form

Row combinations used to annihilate entries above as well as below diagonal

Elimination matrix used for given column vector $\boldsymbol{a}$ of form

$$\begin{bmatrix} 1 & \cdots & 0 & -m_1 & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 1 & -m_{k-1} & 0 & \cdots & 0 \\ 0 & \cdots & 0 & 1 & 0 & \cdots & 0 \\ 0 & \cdots & 0 & -m_{k+1} & 1 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & -m_n & 0 & \cdots & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ \vdots \\ a_{k-1} \\ a_k \\ a_{k+1} \\ \vdots \\ a_n \end{bmatrix} = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ a_k \\ 0 \\ \vdots \\ 0 \end{bmatrix},$$

where $m_i = a_i/a_k$, $i = 1, \ldots, n$

Gauss-Jordan Elimination, cont.

Gauss-Jordan elimination requires about $n^3/2$ multiplications and similar number of additions, 50% more expensive than LU factorization

During elimination phase, same row operations also applied to right-hand-side vector (or vectors) of system of linear equations

Once matrix in diagonal form, components of solution computed by dividing each entry of transformed right-hand-side by corresponding diagonal entry of matrix

Latter requires only n divisions, but not enough cheaper to offset more costly elimination phase

Solving Modified Problems

If right-hand side of linear system changes but matrix does not, then LU factorization need not be repeated to solve new system

Substantial savings in work, since additional triangular solutions cost only $\mathcal{O}(n^2)$ work, in contrast to $\mathcal{O}(n^3)$ cost of factorization

Sometimes refactorization can be avoided even when matrix does change

Sherman-Morrison formula gives inverse of matrix resulting from rank-one change to matrix whose inverse is already known:

$$(\boldsymbol{A}-\boldsymbol{u}\boldsymbol{v}^T)^{-1} = \boldsymbol{A}^{-1}+\boldsymbol{A}^{-1}\boldsymbol{u}(1-\boldsymbol{v}^T\boldsymbol{A}^{-1}\boldsymbol{u})^{-1}\boldsymbol{v}^T\boldsymbol{A}^{-1},$$

where $\boldsymbol{u}$ and $\boldsymbol{v}$ are n-vectors

Evaluation of formula requires $\mathcal{O}(n^2)$ work (for matrix-vector multiplications) rather than $\mathcal{O}(n^3)$ work required for inversion

Solving Modified Problems, cont.

To solve linear system $(\boldsymbol{A} - \boldsymbol{u}\boldsymbol{v}^T)\boldsymbol{x} = \boldsymbol{b}$ with new matrix, use formula to obtain

$$\begin{aligned}\boldsymbol{x} &= (\boldsymbol{A} - \boldsymbol{u}\boldsymbol{v}^T)^{-1}\boldsymbol{b} \\ &= \boldsymbol{A}^{-1}\boldsymbol{b} + \boldsymbol{A}^{-1}\boldsymbol{u}(1 - \boldsymbol{v}^T\boldsymbol{A}^{-1}\boldsymbol{u})^{-1}\boldsymbol{v}^T\boldsymbol{A}^{-1}\boldsymbol{b},\end{aligned}$$

which can be implemented by steps

1. Solve $\boldsymbol{A}\boldsymbol{z} = \boldsymbol{u}$ for $\boldsymbol{z}$, so $\boldsymbol{z} = \boldsymbol{A}^{-1}\boldsymbol{u}$
2. Solve $\boldsymbol{A}\boldsymbol{y} = \boldsymbol{b}$ for $\boldsymbol{y}$, so $\boldsymbol{y} = \boldsymbol{A}^{-1}\boldsymbol{b}$
3. Compute $\boldsymbol{x} = \boldsymbol{y} + ((\boldsymbol{v}^T\boldsymbol{y})/(1 - \boldsymbol{v}^T\boldsymbol{z}))\boldsymbol{z}$

If $\boldsymbol{A}$ already factored, procedure requires only triangular solutions and inner products, so only $\mathcal{O}(n^2)$ work and no explicit inverses

Example: Rank-1 Updating of Solution

Consider rank-one modification

$$\begin{bmatrix} 2 & 4 & -2 \\ 4 & 9 & -3 \\ -2 & -1 & 7 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 2 \\ 8 \\ 10 \end{bmatrix}$$

(with $3,2$ entry changed) of system whose LU factorization was computed in earlier example

One way to choose update vectors:

$$\boldsymbol{u} = \begin{bmatrix} 0 \\ 0 \\ -2 \end{bmatrix} \quad \text{and} \quad \boldsymbol{v} = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix},$$

so matrix of modified system is $\boldsymbol{A} - \boldsymbol{u}\boldsymbol{v}^T$

Example Continued

Using LU factorization of $\boldsymbol{A}$ to solve $\boldsymbol{Az} = \boldsymbol{u}$ and $\boldsymbol{Ay} = \boldsymbol{b}$,

$$\boldsymbol{z} = \begin{bmatrix} -3/2 \\ 1/2 \\ -1/2 \end{bmatrix} \quad \text{and} \quad \boldsymbol{y} = \begin{bmatrix} -1 \\ 2 \\ 2 \end{bmatrix}$$

Final step computes updated solution

$$\boldsymbol{x} = \boldsymbol{y} + \frac{\boldsymbol{v}^T\boldsymbol{y}}{1 - \boldsymbol{v}^T\boldsymbol{z}}\boldsymbol{z} =$$

$$\begin{bmatrix} -1 \\ 2 \\ 2 \end{bmatrix} + \frac{2}{1 - 1/2}\begin{bmatrix} -3/2 \\ 1/2 \\ -1/2 \end{bmatrix} = \begin{bmatrix} -7 \\ 4 \\ 0 \end{bmatrix}$$

We have thus computed solution to modified system without factoring modified matrix

Scaling Linear Systems

In principle, solution to linear system unaffected by diagonal scaling of matrix and right-hand-side vector

In practice, scaling affects both conditioning and selection of pivots in Gaussian elimination, which in turn affect numerical accuracy in finite-precision arithmetic

Usually best if all entries (or uncertainties in entries) of matrix have about same size

Sometimes obvious how to accomplish this by choice of measurement units for variables, but there is no foolproof method for doing so in general

Scaling can introduce rounding errors if not done carefully

Example: Scaling

Linear system

$$\begin{bmatrix} 1 & 0 \\ 0 & \epsilon \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 1 \\ \epsilon \end{bmatrix}$$

has condition number $1/\epsilon$, so ill-conditioned if ϵ small

If second row multiplied by $1/\epsilon$, then system becomes perfectly well-conditioned

Apparent ill-conditioning due purely to poor scaling

Much less obvious how to correct poor scaling in general

Iterative Refinement

Given approximate solution $\boldsymbol{x}_0$ to linear system $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$, compute residual

$$\boldsymbol{r}_0 = \boldsymbol{b} - \boldsymbol{A}\boldsymbol{x}_0$$

Now solve linear system $\boldsymbol{A}\boldsymbol{z}_0 = \boldsymbol{r}_0$ and take

$$\boldsymbol{x}_1 = \boldsymbol{x}_0 + \boldsymbol{z}_0$$

as new and "better" approximate solution, since

$$\begin{aligned} \boldsymbol{A}\boldsymbol{x}_1 &= \boldsymbol{A}(\boldsymbol{x}_0 + \boldsymbol{z}_0) = \boldsymbol{A}\boldsymbol{x}_0 + \boldsymbol{A}\boldsymbol{z}_0 \\ &= (\boldsymbol{b} - \boldsymbol{r}_0) + \boldsymbol{r}_0 = \boldsymbol{b} \end{aligned}$$

Process can be repeated to refine solution successively until convergence, potentially producing solution accurate to full machine precision

Iterative Refinement, continued

Iterative refinement requires double storage, since both original matrix and LU factorization required

Due to cancellation, residual usually must be computed with higher precision for iterative refinement to produce meaningful improvement

For these reasons, iterative improvement often impractical to use routinely, but can still be useful in some circumstances

Special Types of Linear Systems

Work and storage can often be saved in solving linear system if matrix has special properties

Examples include:

- Symmetric: $\boldsymbol{A} = \boldsymbol{A}^T$, $a_{ij} = a_{ji}$ for all i, j
- Positive definite: $\boldsymbol{x}^T \boldsymbol{A} \boldsymbol{x} > 0$ for all $\boldsymbol{x} \neq \boldsymbol{o}$
- Band: $a_{ij} = 0$ for all $|i - j| > \beta$, where β is *bandwidth* of $\boldsymbol{A}$
- Sparse: most entries of $\boldsymbol{A}$ are zero

Symmetric Positive Definite Matrices

If $\boldsymbol{A}$ is symmetric and positive definite, then LU factorization can be arranged so that

$$\boldsymbol{U} = \boldsymbol{L}^T, \quad \text{that is,} \quad \boldsymbol{A} = \boldsymbol{L}\boldsymbol{L}^T,$$

where $\boldsymbol{L}$ is lower triangular with positive diagonal entries

Algorithm for computing *Cholesky factorization* derived by equating corresponding entries of $\boldsymbol{A}$ and $\boldsymbol{L}\boldsymbol{L}^T$ and generating them in correct order

In 2×2 case, for example,

$$\begin{bmatrix} a_{11} & a_{21} \\ a_{21} & a_{22} \end{bmatrix} = \begin{bmatrix} l_{11} & 0 \\ l_{21} & l_{22} \end{bmatrix} \begin{bmatrix} l_{11} & l_{21} \\ 0 & l_{22} \end{bmatrix},$$

which implies

$$l_{11} = \sqrt{a_{11}}, \quad l_{21} = a_{21}/l_{11}, \quad l_{22} = \sqrt{a_{22} - l_{21}^2}$$

Cholesky Factorization

One way to write resulting general algorithm, in which Cholesky factor $\boldsymbol{L}$ overwrites original matrix $\boldsymbol{A}$:

```
for j = 1 to n
    for k = 1 to j − 1
        for i = j to n
            a_ij = a_ij − a_ik · a_jk
        end
    end
    a_jj = sqrt(a_jj)
    for k = j + 1 to n
        a_kj = a_kj / a_jj
    end
end
```

for $j = 1$ **to** n
    for $k = 1$ **to** $j - 1$
        for $i = j$ **to** n
            $a_{ij} = a_{ij} - a_{ik} \cdot a_{jk}$
        end
    end
    $a_{jj} = \sqrt{a_{jj}}$
    for $k = j + 1$ **to** n
        $a_{kj} = a_{kj}/a_{jj}$
    end
end

Cholesky Factorization, continued

Features of Cholesky algorithm symmetric positive definite matrices:

- All n square roots are of positive numbers, so algorithm well defined
- No pivoting required for numerical stability
- Only lower triangle of $\boldsymbol{A}$ accessed, and hence upper triangular portion need not be stored
- Only $n^3/6$ multiplications and similar number of additions required

Symmetric Indefinite Systems

For symmetric indefinite $\boldsymbol{A}$, Cholesky factorization not applicable, and some form of pivoting generally required for numerical stability

Factorization of form

$$\boldsymbol{P}\boldsymbol{A}\boldsymbol{P}^T = \boldsymbol{L}\boldsymbol{D}\boldsymbol{L}^T,$$

with $\boldsymbol{L}$ unit lower triangular and $\boldsymbol{D}$ either tridiagonal or block diagonal with 1×1 and 2×2 diagonal blocks, can be computed stably using symmetric pivoting strategy

In either case, cost comparable to Cholesky factorization

Band Matrices

Gaussian elimination for band matrices differs little from general case — only ranges of loops change

Typically store matrix in array by diagonals to avoid storing zero entries

If pivoting required for numerical stability, bandwidth can grow (but no more than double)

General purpose solver for arbitrary bandwidth similar to code for Gaussian elimination for general matrices

For fixed small bandwidth, band solver can be extremely simple, especially if pivoting not required for stability

Tridiagonal Matrices

Consider tridiagonal matrix, for example

$$\boldsymbol{A} = \begin{bmatrix} b_1 & c_1 & 0 & \cdots & 0 \\ a_2 & b_2 & c_2 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & a_{n-1} & b_{n-1} & c_{n-1} \\ 0 & \cdots & 0 & a_n & b_n \end{bmatrix}$$

If pivoting not required for stability, then Gaussian elimination reduces to

$d_1 = b_1$
for $i = 2$ **to** n
    $m_i = a_i/d_{i-1}$
    $d_i = b_i - m_i c_{i-1}$
end

Tridiagonal Matrices, continued

LU factorization of $\boldsymbol{A}$ given by

$$\boldsymbol{L} = \begin{bmatrix} 1 & 0 & \cdots & \cdots & 0 \\ m_2 & 1 & \ddots & & \vdots \\ 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & m_{n-1} & 1 & 0 \\ 0 & \cdots & 0 & m_n & 1 \end{bmatrix},$$

$$\boldsymbol{U} = \begin{bmatrix} d_1 & c_1 & 0 & \cdots & 0 \\ 0 & d_2 & c_2 & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ \vdots & & \ddots & d_{n-1} & c_{n-1} \\ 0 & \cdots & \cdots & 0 & d_n \end{bmatrix}$$

General Band Matrices

In general, band system of bandwidth β requires $\mathcal{O}(\beta n)$ storage and factorization requires $\mathcal{O}(\beta^2 n)$ work

Compared with full system, savings substantial if $\beta \ll n$

Iterative Methods for Linear Systems

Gaussian elimination is direct method for solving linear system, producing exact solution in finite number of steps (in exact arithmetic)

Iterative methods begin with initial guess for solution and successively improve it until desired accuracy attained

In theory, might take infinite number of iterations to converge to exact solution, but in practice terminate iterations when residual as small as desired

For some types of problems, iterative methods have significant advantages over direct methods

We will study specific iterative methods later when we consider solution of partial differential equations

LINPACK and LAPACK

`LINPACK` is software package for solving wide variety of systems of linear equations, both general dense systems and special systems, such as symmetric or banded

Solving linear systems of such fundamental importance in scientific computing that `LINPACK` has become standard benchmark for comparing performance of computers

`LAPACK` is more recent replacement for `LINPACK` featuring higher performance on modern computer architectures, including some parallel computers

Both `LINPACK` and `LAPACK` available from `Netlib`

Basic Linear Algebra Subprograms

High-level routines in LINPACK and LAPACK based on lower-level Basic Linear Algebra Subprograms (BLAS)

BLAS encapsulate basic operations on vectors and matrices so they can be optimized for given computer architecture while high-level routines that call them remain portable

Generic Fortran versions of BLAS available from Netlib, and many computer vendors provide custom versions optimized for their particular systems

Examples of BLAS

Level	Work	Examples	Function
1	$\mathcal{O}(n)$	`saxpy`	Scalar $\times$ vector $+$ vector
		`sdot`	Inner product
		`snrm2`	Euclidean vector norm
2	$\mathcal{O}(n^2)$	`sgemv`	Matrix-vector product
		`strsv`	Triangular solution
		`sger`	Rank-one update
3	$\mathcal{O}(n^3)$	`sgemm`	Matrix-matrix product
		`strsm`	Multiple triang. solutions
		`ssyrk`	Rank-k update

Level-3 `BLAS` have more opportunity for data reuse, and hence higher performance, because they perform more operations per data item than lower-level `BLAS`