Numerical Analysis - Math 464 and 465 Notes

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1 Floating Point and Roundoff Error

1.1 Number Representation

Definition 1.1. Let $\beta > 1$ be an integer. We call β the *base* of a number system. Let a_k, b_k be integers such that $0 \leq a_k, b_k < \beta$. Then any real number x can be represented by

$$x = (a_n\, a_{n-1} \cdots a_1\, a_0\, .\, b_1\, b_2\, b_3 \cdots)_\beta\,.$$

We call the dot between a_0 and b_1 the *radix point*. Alternatively, we can represent x by two summations:

$$x = a_k\beta^k + a_{k-1}\beta^{k-1} + \cdots + a_1\beta + a_0 + b_1\beta^{-1} + b_2\beta^{-2} + \cdots = \sum_{k=0}^{n} a_k\beta^k + \sum_{k=1}^{\infty} b_k\beta^{-k}$$

We call the first sum the *integral part of* x and denote it by x_I, and the second sum the *fractional part of* x and denote it by x_F. We call for formulas above the *expansion* of x.

Definition 1.2. An expansion of some real number x is said to *terminate* if there exists some $K \geq 0$ such that $b_k = 0$ for all $k \geq K$.

Theorem 1.3. A real number x has a terminating expansion in base β if and only if x is rational and when x is expressed in simplest form, the only prime factors of the denominator of x are factors of β.

Theorem 1.4. Let x be a real number. If x does not have a terminating expansion in base β, then the expansion of x in base β is unique. If $x \neq 0$, has a terminating expansion in base β, then it has exactly on terminating expansion (ending in zeros) and exactly one nonterminating expansion (ending in $(\beta - 1)$'s).

Remark.

(i) The expansions of negative numbers are just prefixed by a minus sign, e.g. $-1/8 = -(0.12500\cdots)_{10}$.

(ii) There are algorithms for converting expansions from one case to another.

1.2 Normalized Scientific Notation in Base β

Lemma 1.5. Let $\beta > 1$ be an integer. For any real number $x > 0$, there is a unique integer c and a unique number $r \in [1/\beta, 1)$ so that $x = r\beta^c$. The number r can be expressed as an expansion in base β,

$$r = (.\, d_1\, d_2\, d_3 \cdots)_\beta$$

with $d_1 \neq 0$.

Theorem 1.6. Let $x \neq 0$ be any real number. Then x has an expansion in base β,

$$x = \pm\,(.\, d_1\, d_2\, d_3 \cdots)_\beta\, \beta^c$$

with $d_1 \neq 0$.

Definition 1.7. The representation of x in Theorem 1.6 is called the *normalized scientific notation* for x in base β. It is unique, except for real numbers x with terminating expansions (which have two expansions); we always choose the terminating expansion.

1.3 Floating Point Arithmetic

Definition 1.8. An *m-digit floating-point number in base* β is denoted by

$$x = \pm \left(. \, d_1 \, d_2 \cdots d_m\right)_\beta \beta^c$$

where $\left(. \, d_1 \, d_2 \cdots d_m\right)_\beta$ is called the *mantissa* and c is called the exponent. If $d_1 \neq 0$ (or $x = 0$), called a *normalized floating-point number.*

Remark. In computers, the base is usually $\beta = 2$ and mantissa lengths usually comes in two sizes: single (23) and double (52). Additionally, the exponent c has a limited range $-M \leq c \leq M$.

Definition 1.9. Any real number can be represented approximately by floating-point numbers. For every real number x, the floating-point value $\text{fl}(x)$ is the approximate value of x. Generally, fl is only well defined for some domain $\{x : \beta^{\mu-1} \leq |x| < \beta^M\}$. Otherwise, *underflow* or *overflow* occurs.

Definition 1.10. The function fl is commonly defined in two different ways:

(i) *Rounding* - $\text{fl}(x)$ is the normalized floating-point number closest fo x. In case of a tie, round to an even digit (symmetric rounding about 0).

(ii) *Truncating* - $\text{fl}(x)$ is the nearest normalized floating-point number between x and 0.

Remark. A more precise definition of the fl functions exists for even β. Let $x = \pm r\beta^c$ be a real number in normalized scientific notation where

$$r = (0 \, . \, d_1 \, d_2 \, d_3 \cdots)$$

Then $\text{fl}(x)$ for an m-digit floating-point representation with a maximum M exponent is

$$\text{fl}(x) = \begin{cases} 0, & x = 0 \\ \text{underflow}, & 0 < |x| < \beta^{\mu-1} \text{ (possibly extended to } \beta^{\mu-m} \leq |x| < \beta^{\mu-1}) \\ \text{overflow}, & |x| \geq \beta^M \\ \pm(. \, d_1 \, d_2 \cdots d_m)_\beta \beta^c, & \text{truncating} \\ \pm(. \, d_1 \, d_2 \cdots d_m)_\beta \beta^c, & \text{rounding, } (\, d_{m+1} \, d_{m+2} \cdots) < 1/2 \\ \pm\left[(. \, d_1 \, d_2 \cdots d_m)_\beta + (.00 \cdots 1)_\beta\right] \beta^c, & \text{rounding, } (\, d_{m+1} \, d_{m+2} \cdots) > 1/2 \\ \pm\left[(. \, d_1 \, d_2 \cdots d_m)_\beta + (.00 \cdots 1)_\beta\right] \beta^c, & \text{rounding, } (\, d_{m+1} \, d_{m+2} \cdots) = 1/2, d_m \text{ is odd} \\ \pm\left[(. \, d_1 \, d_2 \cdots d_m)_\beta - (.00 \cdots 1)_\beta\right] \beta^c, & \text{rounding, } (\, d_{m+1} \, d_{m+2} \cdots) = 1/2, d_m \text{ is even} \end{cases}$$

1.4 Absolute and Relative Error

Definition 1.11. Suppose that x' is an approximation to a real number x. Then the *absolute error in* x' is $x - x'$ and the *relative error in* x' (if $x \neq 0$) is $(x - x')/x$.

Definition 1.12. The *roundoff error* is the error in $\text{fl}(x)$ as an approximation to x. Usually it is absolute error $x - \text{fl}(x)$.

Theorem 1.13. Suppose $\beta^{\mu-1} \leq |x| < \beta^M$. Define $\delta = \delta(x) = (\text{fl}(x) - x)/x$ to be the relative error of $\text{fl}(x)$.

(i) For rounding, $|\delta| \leq \beta^{1-m}/2$.

(ii) For truncating, $-\beta^{1-m} < \delta \leq 0$.

Definition 1.14. The maximum possible value for $|\delta|$ when there is no underflow or overflow is called the *unit roundoff*, denoted by u. In rounding, $u = \beta^{1-m}/2$. In truncating, $u = \beta^{1-m}$.

Remark. The value $\delta = (\text{fl}(x) - x)/x$ can be rearranged to form $\text{fl}(x) = x(1+\delta)$. This is useful in error analysis. If we define $\varepsilon(x) = (\text{fl}(x) - x)/\text{fl}(x)$, then $|\varepsilon| < \beta^{1-m}/2$ for rounding and $|\varepsilon| < \beta^{1-m}$ for truncating. Here, $\text{fl}(x) = x/(1+\epsilon)$.

Definition 1.15. The *machine epsilon* is defined to be $\varepsilon = \sup\{y > 0 : \text{fl}(1+y) = 1\}$.

Remark. The machine epsilon can also be defined to be $\varepsilon = \inf\{y > 0 : \text{fl}(1+y) > 1\}$. The machine epsilon is exactly the same as the unit roundoff.

1.5 Arithmetic Operations with Floating-Point Numbers

Definition 1.16. With β, m fixed, the set of floating-point numbers is not closed under the usual operations $+$, $-$, $\times$, and $\div$. Machines are usually constructed so that

$$x \circ^* y = \text{fl}(x \circ y).$$

where $\circ$ is $+$, $-$, $\times$, or $\div$, and $\circ^*$ is the corresponding *floating-point operation*. Unless underflow or overflow occurs

$$x \circ^* y = (x \circ y)(1+\delta)$$

for some δ where $\delta \leq u$ where x, y are floating-point numbers. Alternatively,

$$x \circ^* y = (x \circ y)/(1+\varepsilon)$$

for some ε where $|\varepsilon| \leq \mu$.

Theorem 1.17. Suppose $0 < u < 1$ and $|\delta_j| \leq u$ for $j = 1, \ldots, r$. Then there exists a δ with $|\delta| \leq u$ such that

$$(1+\delta_1)\cdots(1+\delta_r) = (1+\delta)^r$$

Corollary 1.18. For the theorem above, if $ru \ll 1$, then $(1+\delta)^r \approx 1 + r\delta$.

Remark. For two real number p, q, the operation $\text{fl}(p) \times \text{fl}(q)$ is

$$\text{fl}(p) \times \text{fl}(q) = pq(1+\delta_1)(1+\delta_2)(1+\delta_3) = pq(1+\delta)^3.$$

This kind of analysis is called backward error analysis.

Definition 1.19. Suppose x is written in normalized scientific notation in base β,

$$x = (.\, d_1\, d_2\, d_3 \cdots)_\beta \beta^c$$

where $d_1 \neq 0$. The digit d_j is called the *j-th significant digit* of x; d_j is the coefficient of β^{c-j}.

Definition 1.20. Suppose x' is an approximation to x. If $|x - x'| \leq \beta^{c-r}/2$, we say x' *approximates x to r significant digits*. Very approximately, the number of significant digits in x' is $-\log_\beta |(x - x')/x|$.

Theorem 1.21. Very approximately, if x and y have t significant digits, have the same sign, and agree to s significant digits, then the computed value of $x - y$ will have only $t - s$ significant digits.

Theorem 1.22. Let $x_1, x_2, \ldots, x_{n+1}$ be positive normalized floating-point numbers, $+$ be true addition, $\bigoplus$ be machine addition, u be the unit roundoff with $0 < u < 1$, and assume no overflow when we add $x_1, \ldots, x_{n+1}$. Then there are numbers $\delta_1, \ldots, \delta_n$ with $|\delta_j| \leq u$ for which

(i) $x_1 \bigoplus x_2 = (x_1 + x_2)(1 + \delta_1)$

(ii) $(x_1 \bigoplus x_2) \bigoplus x_3 = (x_1 + x_2)(1 + \delta_1)(1 + \delta_2) + x_3(1 + \delta_2)$

(iii) $x_1 \bigoplus x_2 \bigoplus \cdots \bigoplus x_{n+1} = (x_1 + x_2)(1 + \delta_1)\cdots(1 + \delta_n) + x_3(1 + \delta_2)\cdots(1 + \delta_n) + \cdots + x_{n+1}(1 + \delta_n)$

Remark. Consider solving $ax^2 + bx + c = 0$ by the quadratic formula when $ac \neq 0$, $b \neq 0$, and $b^2 - 4ac > 0$. The two solutions can be each written in two ways:

$$\frac{-b + \sqrt{b^2 - 4ac}}{2a} = \left(\frac{-b + \sqrt{b^2 - 4ac}}{2a}\right)\left(\frac{-b - \sqrt{b^2 - 4ac}}{-b - \sqrt{b^2 - 4ac}}\right) = \frac{4ac}{2a(-b - \sqrt{b^2 - 4ac})} = \frac{2c}{-b - \sqrt{b^2 - 4ac}},$$

and similarly,

$$\frac{-b - \sqrt{b^2 - 4ac}}{2a} = \frac{2c}{-b + \sqrt{b^2 - 4ac}}.$$

When $b > 0$, $-b + \sqrt{b^2 - 4ac}$ could have cancellation, and when $b < 0$, $-b - \sqrt{b^2 - 4ac}$ could have cancellation. Thus a better implementation of the quadratic formula is when $b > 0$, the two roots are $2c/(-b - \sqrt{b^2 - 4ac})$ and $(-b - \sqrt{b^2 - 4ac})/2a$, and when $b < 0$, the two roots are $(-b + \sqrt{b^2 - 4ac})/2a$ and $2c/(-b + \sqrt{b^2 - 4ac})$.

1.6 Converting Between Bases

Theorem 1.23. Suppose $N = (a_n\, a_{n-1} \cdots a_0)_\alpha$ is represented in base α. The expansion of N in base β can be found using two different methods:

(i) Express $\alpha, a_0, a_1, \cdots, a_n$ in base β. Then N is

$$N = (((a_n \cdot \alpha + a_{n-1}) \cdot \alpha + \cdots) \cdot \alpha + a_1) \cdots \alpha + a_0$$

where each operation is in base β arithmetic.

(ii) Suppose $N = (c_m\, c_{m-1} \cdots c_0)_\beta$. Then

$$N = c_0 + \beta \cdot (c_1 + \beta \cdot (c_2 + \cdots)).$$

Theorem 1.24. Suppose $x = (.\, b_1\, b_2 \cdots b_m)_\alpha$ is represented in base α. The expansion of x in base β can be found using two different methods:

(i) Express $\alpha, b_1, b_2 \cdots, b_m$ in base β. Then N is

$$N = (((b_m/\alpha + b_{m-1})/\alpha + \cdots + b_2)/\alpha + b_1)/\alpha$$

where each operation is in base β arithmetic.

(ii) Suppose $N = (c_m\, c_{m-1} \cdots c_0)_\beta$. The expansion of x can be found by successively solving for each coefficient in base β. Let $x = (.\, c_1\, c_2 \cdots)_\beta$ for unknown coefficients $c_1, c_2, \ldots$.

$$\begin{aligned} \beta x &= (c_1\, .\, c_2\, c_3 \cdots)_\beta, \quad \text{so} \quad c_1 = (\beta x)_I \\ \beta(\beta x)_F &= (c_2\, .\, c_3\, c_4 \cdots)_\beta, \quad \text{so} \quad c_2 = (\beta(\beta x)F)_I \\ &\vdots \end{aligned}$$

2 Solutions of Linear Systems

2.1 Solutions of Linear Systems using Elimination

Definition 2.1. Consider the matrix equation $A\mathbf{x} = \mathbf{b}$ where A is an upper triangular matrix whose diagonal entires are all non-zero, that is,

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n &= b_1 \\ a_{22}x_2 + \cdots + a_{2n}x_n &= b_2 \\ &\vdots \\ a_{nn}x_n &= b_n \end{aligned}$$

To solve for $\mathbf{x}$, begin with x_n: $x_n = b_n/a_{nn}$. Then solve for x_{n-1}: $x_{n-1} = (b_{n-1} - a_{n-1,n}x_n)/a_{n-1,n-1}$. In general,

$$x_k = \frac{b_k - \sum_{j=k+1}^{n} a_{kj}x_j}{a_{kk}}.$$

This method of solving is called *back subtitution*.

Theorem 2.2. An upper triangular matrix A is invertible if and only if all diagonal entries are non-zero.

Definition 2.3. For any matrix equation $A\mathbf{x} = \mathbf{b}$ where A is a square matrix, the method of solving for $\mathbf{x}$ by transforming the equation into an equivalent equation where the matrix is an upper triangular matrix is called *Gaussian elimination*. This transformation requires finding a sequence of equivalent linear systems

$$A^{(k)}\mathbf{x} = \mathbf{b}^{(k)}, \quad 0 \le k \le n-1$$

where $A^{(0)} = A, \mathbf{b}^{(0)} = \mathbf{b}$ and $A^{(n-1)}$ is an upper triangular matrix. The i-th equation and $(i+1)$-th equation is separated by a single row operation.

Remark. Fix $k > 1$ (the case $k - 1 = 0$ is trivial). If $a_{kk}^{(k-1)} \neq 0$, add a multiple $-a_{ik}^{(k-1)}/a_{kk}^{k-1}$ of k-th row to the i-th row for $i = k+1, \ldots, n$. Then $a_{ik}^{k} = 0$ for $i = k+1, \ldots, n$.

Remark. The value $m_{ik} = a_{ik}^{(k-1)}/a_{kk}^{(k-1)}$ gets stored in the ik-position (if no pivoting).

Definition 2.4. Assuming no pivoting is necessary, Gaussian elimination reduces to

$$A^{n-1} = M_{n-1} \cdots M_1 A^{(0)}.$$

where $m_{ik} = a_{ik}^{(k-1)}/a_{kk}^{(k-1)}$ and

$$M_k = \begin{bmatrix} 1 & & & & 0 \\ & 1 & & & \\ & & 1 & & \\ & & -m_{k+1,k} & 1 & \\ & & \vdots & \ddots & \\ 0 & & -m_{n,k} & 0 & 1 \end{bmatrix}.$$

Let $U = A^{(n-1)}$. U is upper triangular with non-zero diagonal elements. Then

$$A = M_1^{-1} M_2^{-1} \cdots M_{n-1}^{-1} U.$$

Now,

$$M_k^{-1} = \begin{bmatrix} 1 & & & & 0 \\ & 1 & & & \\ & & 1 & & \\ & & m_{k+1,k} & 1 & \\ & & \vdots & \ddots & \\ 0 & & m_{n,k} & 0 & 1 \end{bmatrix}.$$

Let $L = M_1^{-1} M_2^{-1} \cdots M_{n-1}^{-1}$. Then

$$L = \begin{bmatrix} 1 & & & & \\ m_{21} & 1 & & & \\ m_{31} & m_{32} & 1 & & \\ \vdots & \vdots & & \ddots & \\ m_{n1} & m_{n2} & \cdots & \cdots & 1 \end{bmatrix}.$$

and $A = LU$. The product LU the *LU factorization of A*. The matrix L is a unit lower-triangular matrix.

Remark. Let $\mathbf{y}$ be the solution of $L\mathbf{y} = \mathbf{b}$. Since $L = M_1^{-1} M_2^{-1} \cdots M_{n-1}^{-1}$,

$$y = M_{n-1} \cdots M_1 \mathbf{b}.$$

Solving for $\mathbf{y}$ is equivalent to performing elimination steps on $\mathbf{b}$. Then we only need to solve $U\mathbf{x} = \mathbf{y}$ to obtain $\mathbf{x}$. Since $\mathbf{x}$ is upper-triangular we only need to perform back subtitution.

Consider solving $A\mathbf{x} = \mathbf{b}$ for an $n \times n$ matrix using Gaussian elimination.

Step	Multiplies (Scaling)	Multiplies (Elimination)	Additions (Eliminations)
$A^{(0)} \to A^{(1)}$	$n-1$	$(n-1)^2$	$(n-1)^2$
$A^{(1)} \to A^{(2)}$	$n-2$	$(n-2)^2$	$(n-2)^2$
$\vdots$	$\vdots$	$\vdots$	$\vdots$
$A^{(n-3)} \to A^{(n-2)}$	2	4	4
$A^{(n-2)} \to A^{(n-1)}$	1	1	1

The total number of multiplication operations is

$$\sum_{j=1}^{n-1} j + \sum_{j=1}^{n-1} j^2 = \frac{n(n-1)}{2} + \frac{n(n-1)(2n-1)}{6} \approx \frac{1}{3}n^3$$

while the total number of additions is

$$\sum_{j=1}^{n-1} j^2 = \frac{n(n-1)(2n-1)}{6} \approx \frac{1}{3}n^3.$$

Thus the total number of operations is $2n^3/3$.

Consider instead using the LU-factorization of A. For the forward elimination step ($L\mathbf{y} = \mathbf{b}$),

Solving	Multiplies	Additions
$\mathbf{y}_2$	1	1
$\mathbf{y}_3$	2	2
$\vdots$	$\vdots$	$\vdots$
$\mathbf{y}_{n-1}$	$n-2$	$n-2$
$\mathbf{y}_n$	$n-1$	$n-1$

the total number of operations is

$$\sum_{j=1}^{n-1} j + \sum_{j=1}^{n-1} j = \frac{n(n-1)}{2} + \frac{n(n-1)}{2} \approx n^2.$$

For the back substitution step,

Solving	Multiplies	Additions
$\mathbf{x}_n$	1	0
$\mathbf{x}_{n-1}$	2	1
$\vdots$	$\vdots$	$\vdots$
$\mathbf{x}_2$	$n-1$	$n-2$
$\mathbf{x}_1$	n	$n-1$

the total number of operations is

$$\sum_{j=1}^{n} j + \sum_{j=0}^{n-1} j = \frac{n(n+1)}{2} + \frac{n(n-1)}{2} \approx n^2.$$

Therefore, the LU-factorization method requires $2n^2$ operations.

2.2 Pivoting

Definition 2.5. In elimination, a *pivotal equation* is the equation used to elimination an unknown from the other equations. At the start of the k-th elimination step, a pivotal equation is the equation with a non-zero coefficient for x_k in the k-th, $k+1$-th, ..., n-th equations.

Theorem 2.6. A is invertible if and only if there is at least one pivotal equation at every elimination step.

Remark. Pivoting can be viewed as multiplying A by a permutation matrix $P^\top$, and then finding the LU-factorization of $P^\top A$. Then, $A = PLU$.

Theorem 2.7. Every invertible matrix A can be written as a product PLU where P is a permutation matrix, L is a unit lower-triangular matrix and U is an (invertible) upper triangular matrix.

Theorem 2.8. An invertible matrix A has an LU-factorization if and only if each of the upper left hand submatrices

$$A_k = \begin{bmatrix} a_{11} & \dots & a_{1k} \\ \vdots & \ddots & \vdots \\ a_{k1} & \dots & a_{kk} \end{bmatrix}$$

for $k = 1, \dots, n$ are invertible.

Remark. In practice, not every pivot equation is good for numerical calculations

(i) Do not choose near-zero pivots.

(ii) Cannot just use absolute comparison of $a_{ik}^{(k-1)}$.

(iii) The best pivot maximizes the ratio of the size of pivot entry to the size of the row.

Remark. Suppose we are on the k-th step of Gaussian Elimination (where $1 \leq k \leq n-1$). The current matrix looks like

$$A^{(k-1)} = \begin{bmatrix} a_{11}^{(k-1)} & & \cdots & & a_{1n}^{(k-1)} \\ & \ddots & & & \\ & & a_{kk}^{(k-1)} & & \vdots \\ & & \vdots & \ddots & \\ & & a_{nk}^{(k-1)} & \cdots & a_{nn}^{(k-1)} \end{bmatrix}.$$

Which entries $a_{kk}^{(k-1)}, \cdots, a_{nk}^{(k-1)}$ should we use as the k-th pivot element?

Definition 2.9. The technique of *simple pivoting* involves choosing the pivot row with the smallest $I \geq k$ for which $A_{Ik}^{(k-1)} \neq 0$, and interchanging the k-th row and the I-th row.

Definition 2.10. The technique of *partial pivoting* involves choosing the pivot row with the entry $\left|a_{Ik}^{(k-1)}\right|$ that is the largest of $\left|a_{kk}^{(k-1)}\right|, \left|a_{k+1,k}^{(k-1)}\right|, \cdots, \left|a_{nk}^{(k-1)}\right|$, and interchanging the k-th row and the I-th row.

Definition 2.11. The technique of *scaled partial pivoting* involves computing scale factors for each row:

$$d_i = \max_{1 \leq j \leq n} |a_{ij}| \quad \text{for} \quad i = 1, \ldots, n$$

before elimination procedure begins and interchanging them when rows are interchanged. At the k-th step, the pivot row for which $a_{Ik}^{(k-1)}/d_I$ is the maximized for all $I \geq k$, is chosen, and the k-th and I-th row are interchanged. Alternatively, the scale factors can be recomputed at every step.

Definition 2.12. In *total pivoting*, the columns are also interchanged. At the k-th step, choose $I \geq k$ and $J \geq k$ for which $|a_{IJ}^{(k-1)}|$ is the maximum of $|a_{ij}|$ for $i = k, \ldots, n$ and $j = k, \ldots, n$. Interchange the k-th row and the I-th row and interchange the k-th column and the J-th column.

Lemma 2.13. The operation counts of each pivoting strategy are as follows:

(i) partial pivoting: $\sum_{k=1}^{(n-1)}(n-k) \approx n^2/2$,

(ii) scaled pivoting (without updating scale factors): $n(n-1) + \sum_{k=1}^{(n-1)}[(n-k+1)+(n-k)] \approx 2n^2$,

(iii) scaled pivoting (updating scale factors): $\sum_{k=1}^{(n-1)}[(n-k+1)(n-k)+(n-k+1)+(n-k)] \approx n^3/3$,

(iv) total pivoting: $\sum_{k=1}^{n-1}\left[(n-k+1)^2-1\right] \approx n^3/3$.

2.3 Interchanging

Theorem 2.14. Let U be an equivalent, upper-triangular form of A, that is,

$$U = (M_{n-1}P_{n-1}) \cdots (M_1 P_1)A,$$

where P_k is either the identity matrix if no interchanging occurs in the k-th step or P_k just interchanges row k with row I for some $I > k$.

Theorem 2.15. Suppose $k > l$ and P_k interchanges rows k and I where $I > k$. Then $P_k M_l = \widetilde{M}_l P_k$ where

$\widetilde{M_l}P$ is the same as M_l except hte multiplies m_{kl} and m_{Il} have been interchanged.

$$P_k = \begin{bmatrix} 1 & & & & \\ & 0 & 1 & & \\ & 1 & 0 & & \\ & & & & 1 \end{bmatrix} \qquad P_k M_l = \begin{bmatrix} 1 & & & & \\ & 1 & & & \\ & m_{Il} & 0 & 1 & \\ & m_{kl} & 1 & 0 & \\ & & & & 1 \end{bmatrix}$$

Definition 2.16. Let the matrix $\hat{M}_l$ be the same as M_l, except all the multiplies in the i-th columns have been interchanged by the P_k's for $k > l$. Then, $U = (\hat{M}_{n-1} \cdots \hat{M}_1)(P_{n-1} \cdots P_1)A = L^{-1}P^\top A$. Then, $A = PLU$. This is called the *PLU factorization* of A. Note that $P^\top A = LU$, so it also encodes the LU factorization of $(P_{n-1} \cdots P_1)A$ which is just A wiht its rows permuted.

3 Norms and Error Analysis

3.1 Vector Norms on $\mathbb{R}^n$ and $\mathbb{C}^n$

Definition 3.1. A *norm* on a vector space is a function that maps a vector, $\mathbf{x} \in \mathcal{V}$, to a number and is denoted by $||\mathbf{x}||$. A norm must satisfy the following properties for all $\mathbf{x}, \mathbf{y} \in \mathcal{F}^n$ and $\alpha \in \mathcal{F}$ where $\mathcal{F}$ is $\mathbb{R}$ or $\mathbb{C}$:

(i) $||\mathbf{x}|| \geq 0$; $||\mathbf{x}|| = 0$ if and only if $\mathbf{x} = \mathbf{0}$,

(ii) $||\alpha\mathbf{x}|| = |\alpha| \cdot ||\mathbf{x}||$,

(iii) $||\mathbf{x} + \mathbf{y}|| \leq ||\mathbf{x}|| + ||\mathbf{y}||$ (triangle inequality).

Remark. Common examples of vector norms include:

(i) $||\mathbf{x}||_1 = \sum_{1 \leq j \leq n} |x_j|$,

(ii) $||\mathbf{x}||_2 = \left(\sum_{j=1}^n |a_j|^2\right)^{1/2}$,

(iii) $||\mathbf{x}||_\infty = \max_{1 \leq j \leq n} |a_j|$.

Definition 3.2. The set of $n \times n$ matrices is itself a vector space. A norm on this vector space satisfies for matrices $A, B \in \mathcal{F}^{n \times n}$ and $\alpha \in \mathcal{F}$ where $\mathcal{F}$ is $\mathbb{R}$ or $\mathbb{C}$:

(i) $||A|| \geq 0$ and $||A|| = 0$ if and only if A is the 0 matrix,

(ii) $||\alpha A|| = |\alpha| \cdot ||A||$,

(iii) $||A + B|| \leq ||A|| + ||B||$.

We call the norm a *matrix norm* if in addition we have

$$||AB|| \leq ||A|| \cdot ||B||.$$

Definition 3.3. Given a vector norm on $\mathbb{R}^n$ (or $\mathbb{C}^n$), the *operator norm induced by vector norm*, or just *operator norm*, on $n \times n$ matrices is

$$||A|| = \sup_{\mathbf{x} \neq \mathbf{0}} \frac{||A\mathbf{x}||}{||\mathbf{x}||}.$$

Informally, this norm gives the maximum stretch factor when $\mathbf{x}$ is mapped through A. For $p = 1, 2, \infty$, we call the operator norm induced by $|| \cdot ||_p$ also $||A||_p$.

Theorem 3.4. For $p = 1$ and $p = \infty$, there are explicit expressions for $||A||_1$ and $||A_\infty||$.

$$||A||_1 = \max_{1 \le j \le n} \sum_{j=1}^{n} |a_{ij}| \qquad ||A||_\infty = \max_{1 \le i \le n} \sum_{j=1}^{n} |a_{ij}|$$

Theorem 3.5. The operator norm $||A||_2$ is the square root of the largest eigenvalue of $A^H A$.

Definition 3.6. We say a matrix norm $||\cdot||_m$ is *compatible* with a vector norm $||\cdot||_v$ if for all $A \in \mathcal{F}^{m \times n}$ and $\mathbf{x} \in \mathcal{F}^n$, $||A\mathbf{x}||_v \le ||A||_m \cdot ||\mathbf{x}||_v$.

Definition 3.7. Define the Frobenius norm of A to be

$$||A||_F = \left(\sum_{i=1}^{n} \sum_{j=1}^{n} |a_{ij}|^2 \right)^{1/2}.$$

Theorem 3.8. The Frobenius norm of A is compatible with $||\mathbf{x}||_2$.

3.2 Residual Error

Definition 3.9. Consider $A\mathbf{x} = \mathbf{b}$. Let $\mathbf{x}$ be the true solution and let $\hat{\mathbf{x}}$ be the approximate solution. Define $\mathbf{e} = \mathbf{x} - \hat{\mathbf{x}}$ be the *error vector* and let $\mathbf{r} = \mathbf{b} - A\hat{\mathbf{x}} = A\mathbf{x} - A\hat{\mathbf{x}} = A\mathbf{e}$ be the *residual vector*.

Theorem 3.10. For all n-vector $\mathbf{y}$ for an invertible matrix A such that $A\mathbf{x} = \mathbf{b}$,

$$\frac{||\mathbf{y}||}{||A^{-1}||} \le ||A\mathbf{y}|| \le ||A|| \cdot ||\mathbf{y}||.$$

Definition 3.11. Define $\kappa(A) = ||A|| \cdot ||A^{-1}||$ to be the *condition number of* A when $\kappa(A) \ge 1$.

Theorem 3.12. The relative error of $||\mathbf{e}||/||\mathbf{x}||$ is as large as $\kappa(A) \cdot ||\mathbf{r}||/||\mathbf{b}||$.

Remark. Method for iteratively solving for the solution of a linear system. Consider the origin matrix A. To find $A\hat{\mathbf{x}}$ set $\mathbf{r} = \mathbf{b} - A\hat{\mathbf{x}}$ and solve $A\mathbf{e} = \mathbf{r}$. Call the computed solution $\hat{\mathbf{e}}$. Then $||\hat{\mathbf{e}}||/||\hat{\mathbf{x}}||$ is approximately $||\mathbf{e}||/||\mathbf{x}||$, e.g. if $||\hat{\mathbf{e}}||/||\hat{\mathbf{x}}|| \approx 10^{-s}$, then we expect $\hat{\mathbf{x}}$ has approximately s significant digits as an approximation to $\hat{\mathbf{x}}$. Also expect that $\hat{\mathbf{e}}$ has s significant digits as an approximation to $\mathbf{e}$, but the absolute error in $\hat{\mathbf{e}}$ is much smaller than the absolute error in $\hat{\mathbf{x}}$. If $||\hat{\mathbf{e}}||/||\hat{\mathbf{x}}||$ sufficienty small, then $\hat{\mathbf{x}} + \hat{\mathbf{e}}$ is the approximate solution. Else set $\hat{\mathbf{x}}' = \hat{\mathbf{x}} + \hat{\mathbf{e}}$ and repeat the procedure. Solving successive systems is not very expensive since elimination required $2/3n^3$ and each solve requires $2n^2$.

Definition 3.13. The method of *backward error analysis* involves considering the approximation to be the exact solution of a perturbed system. Let $\hat{\mathbf{x}}$ be the approximate solution of $A\mathbf{x} = \mathbf{b}$ and consier $\hat{\mathbf{x}}$ to be the exact solution of $\hat{A}\mathbf{x} = \mathbf{b}$ where $\hat{A} = A - E$ for some matrix E. Then a bound on E can be found to analyze its effect on $\hat{\mathbf{x}}$ as an approximation to $\mathbf{x}$.

Theorem 3.14. In general, the bound on the error in $\hat{\mathbf{x}}$ relative to $\hat{\mathbf{x}}$ is

$$\frac{||\mathbf{x} - \hat{\mathbf{x}}||}{||\hat{\mathbf{x}}||} \le \kappa(A) \cdot \frac{||E||}{||A||}.$$

Theorem 3.15. Let $\hat{\mathbf{x}}$ be the computed PLU solution of a linear system and the exact solution of $(A +$

$PE)\hat{\mathbf{x}} = \mathbf{b}$ for some $n \times n$ matrix E. Let $u = n \cdot 1.01 \cdot u$ where u is the unit roundoff. If

$$|e_{ij}| \leq u_n |(P^\top A)_{ij}| + u_n(3 + u_n) \sum_{k=1}^{n} |\hat{l}_{ik}| \cdot |\hat{u}_{kj}$$

then the following is usually true,

$$||E|| \leq n \cdot u \cdot ||A|| \quad \text{and} \quad \frac{||\mathbf{x} - \hat{\mathbf{x}}||}{||\hat{\mathbf{x}}||} \leq \kappa(A) \cdot n \cdot u.$$

Remark. If $\kappa(A)$ is large in the above formula, the system is ill-conditioned, although we must compare to u since this definition changes with precision. Let $s = -\log_\beta(\kappa(A) \cdot n \cdot u)$. Then this method gets us approximately s significant digits in $\hat{\mathbf{x}}$ and each successive iteration gets about s more significant digits.

4 Iterative Methods for Linear Systems

4.1 General Iterative Methods

Definition 4.1 (General Iterative Method). Let M be a real $n \times n$ matrix, and let $\mathbf{x}^{(0)}$ be a vector in $\mathbb{R}^n$. Generate a sequence of vector $\mathbf{x}^{(0)}, \mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \ldots$ by setting

$$\mathbf{x}^{(k+1)} = M\mathbf{x}^{(k)} + \mathbf{g} \quad \text{for} \quad k = 0, 1, 2, \ldots$$

where $\mathbf{g}$ is a given fixed vector in $\mathbb{R}^n$.

Lemma 4.2. If $\mathbf{x}^{(k)} \to \hat{\mathbf{x}}$ as $k \to \infty$, then $\hat{\mathbf{x}} = M\hat{\mathbf{x}} + \mathbf{g}$, so $\hat{\mathbf{x}}$ is a solution of the linear system $(I - M)\hat{\mathbf{x}} = \mathbf{g}$.

Theorem 4.3. Let $||\cdot||$ be a vector norm on $\mathbb{R}^n$, and let $\alpha = ||M||$, the matrix norm of M subordinate to the vector norm $||\cdot||$. Suppose $\alpha = ||M|| < 1$. Then

(i) $I - M$ is invertible,

(ii) For any choice of $\mathbf{x}^{(0)}$, the sequence $\mathbf{x}^{(k)}$ generated by $\mathbf{x}^{(k+1)} = M\mathbf{x}^{(k)} + \mathbf{g}$ converges to $\hat{\mathbf{x}}$, i.e. $\mathbf{x}^{(k)} \to \hat{\mathbf{x}}$ as $k \to \infty$.

(iii) If $\mathbf{e}^{(k)} = \mathbf{x}^{(k)} - \hat{\mathbf{x}}$, then $||\mathbf{e}^{(k)} \leq \alpha^k ||\mathbf{e}^{(0)}$.

This theorem is a special case of the Contraction Mapping Fixed Point Theorem.

Definition 4.4 (Splitting Methods). Choose matrices N and P for which $A = N - P$, and consider the iteration

$$N\mathbf{x}^{(k+1)} = P\mathbf{x}^{(k)} + \mathbf{b} \quad \text{for} \quad k = 0, 1, 2, \ldots.$$

We want to choose N and P so that (i) N is invertible, (ii) $N\mathbf{x} = \mathbf{b}$ is easy to solve, and (iii) $||N^{-1}P|| < 1$ in some norm. Analytically, the iteration is the same as $\mathbf{x}^{(k+1)} = M\mathbf{x}^{(k)} + \mathbf{g}$ where $M = N^{-1}P$ and $\mathbf{g} = N^{-1}\mathbf{b}$ (multiply original iteration by N^{-1}). Each iteration is solving the linear system $N\mathbf{x} = \mathbf{w}$ for $\mathbf{x}^{(k+1)}$ where $\mathbf{w} = P\mathbf{x}^{(k)} + \mathbf{b}$.

Lemma 4.5. For the methods descibed above,

(i) if the iteration converges, i.e. $x^{(k)}$ converges, it converges to a solution of $A\mathbf{x} = \mathbf{b}$,

(ii) if N is invertible and $||N^{-1}P|| < 1$ (in some matrix norm subordinate to a vector norm on $\mathbb{R}^n$), the iteration converges to the unique solution of $A\mathbf{x} = \mathbf{b}$.

Definition 4.6 (Jacobi's Method). Given an $n \times n$ matrix A, let

$$L = \begin{bmatrix} 0 & 0 & \cdots & 0 \\ a_{21} & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & 0 \end{bmatrix}, \qquad D = \begin{bmatrix} a_{11} & 0 & \cdots & 0 \\ 0 & a_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & a_{nn} \end{bmatrix}, \qquad U = \begin{bmatrix} 0 & a_{12} & \cdots & a_{1n} \\ 0 & 0 & \cdots & a_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{bmatrix}.$$

Then $A = L + D + U$. Choose $N = D$ and $P = -(L + U)$. Jacobi's method involves iteratively applying the following

$$D\mathbf{x}^{(k+1)} = -(L + U)\mathbf{x}^{(k)} + \mathbf{b}.$$

This is equivalent to the equation:

$$x_i^{(k+1)} = \left(b_i - \sum_{j<i} d_{ij}\mathbf{x}_j^{(k)} - \sum_{j>i} a_{ij}x_j^{(k)} \right) / a_{ii}$$

for $1 \leq i \leq n$ and $k = 0, 1, \ldots$.

Definition 4.7. A matrix is called *(strictly row) diagonally dominant* if

$$|a_{ii}| > \sum_{j \neq i} |a_{ij}| \qquad \text{for} \qquad 1 \leq i \leq n.$$

Theorem 4.8. If A is diagonally dominant, then Jacobi's Method converges.

Definition 4.9 (Gauss-Seidel). From the decompositon in Jacobi's method, choose $N = D + L$ and $P = -U$ and iteratively compute:

$$(D + L)\mathbf{x}^{(k+1)} = -U\mathbf{x}^{(k)} + \mathbf{b}.$$

In the kth iteration (computing $\mathbf{x}^{(k+1)}$ from $\mathbf{x}^{(k)}$), this system for $\mathbf{x}^{(k+1)}$ is solved by forward substitution.

$$x_i^{(k+1)} = \left(b_i - \sum_{j<i} a_{ij}\mathbf{x}_j^{(k+1)} - \sum_{j>i} a_{ij}x_j^{(k)} \right) / a_{ii}$$

for $1 \leq i \leq n$ and $k = 0, 1, \ldots$.

Remark. For Gauss-Seidel, only one vector is needed to store $\mathbf{x}^{(k)}$ and $\mathbf{x}^{(k+1)}$ since $\mathbf{x}$ can be overwritten in-place.

Theorem 4.10. If A is diagonally dominant, then Gauss-Seidel converges, that is, for any choice of $\mathbf{x}^{(0)}$, the sequence $\mathbf{x}^{(k)}$ generated by $(D + L)\mathbf{x}^{(k+1)} = -U\mathbf{x}^{(k)} + b$ converges to the unique solution of $A\mathbf{x} = \mathbf{b}$.

Definition 4.11. A real $n \times n$ matrix is called *symmetric positive definite*, or just positive definite, if A is symmetric, i.e. $A^\top A$ and for all $\mathbf{x} \neq \mathbf{0}$, $\mathbf{x}^\top A\mathbf{x} > 0$.

Theorem 4.12. A real symmetric $n \times n$ matrix is positive definite if and only if all of its eigenvalues are positive.

Theorem 4.13. If A is symmetic positive definite, then Gauss-Seidel converges.

Remark. Usually Gauss-Seidel converges to the true solution faster than Jacobi's method.

Definition 4.14 (Successive Over-Relaxation (SOR)). This is a variant of Gauss-Seidel. Rewrite the Gauss-Seidel iteration as

$$x_i^{(k+1)} = x_i^{(k)} + \left(b_i - \sum_{j<i} a_{ij} x_j^{(k+1)} - \sum_{j \geq i} a_{ij} x_j^{(k)} \right) / a_{ii}.$$

Fix an ω where $0 < \omega < 2$. The SOR iteration is

$$x_i^{(k+1)} = x_i^{(k)} + \omega \left(b_i - \sum_{j<i} a_{ij} x_j^{(k+1)} - \sum_{j \geq i} a_{ij} x_j^{(k)} \right) / a_{ii}.$$

When $0 < \omega < 1$, it is called under-relaxation; when $\omega = 1$, it is Gauss-Seidel; when $1 < \omega < 2$, it is called over-relaxation. In matrix form,

$$\begin{aligned}
\mathbf{x}^{(k+1)} &= \mathbf{x}^{(k)} + \omega D^{-1} \left(\mathbf{b} - L\mathbf{x}^{(k+1)} - (D+U)\mathbf{x}^{(k)} \right) \\
(D + \omega L)\mathbf{x}^{(k+1)} &= D\mathbf{x}^{(k)} + \omega(\mathbf{b} - (D+U)\mathbf{x}^{(k)}) \\
\mathbf{x}^{(k+1)} &= (D+\omega L)^{-1}((1-\omega)D - \omega U)\mathbf{x}^{(k)} + \omega(D+\omega L)^{-1}\mathbf{b} \\
\mathbf{x}^{(k+1)} &= M_\omega \mathbf{x}^{(k)} + \mathbf{g}_\omega
\end{aligned}$$