# 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 $\beta$ 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 $\beta$ 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 $\beta$.

**Theorem 1.4.** Let $x$ be a real number. If $x$ does not have a terminating expansion in base $\beta$, then the expansion of $x$ in base $\beta$ is unique. If $x \neq 0$, has a terminating expansion in base $\beta$, 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 $\beta$

**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 $\beta$,

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

with $d_1 \neq 0$.

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

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

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 $\beta$. 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* $\beta$ is denoted by

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

where $(.\,d_1\,d_2 \cdots d_m)_\beta$ 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 $\mathrm{fl}(x)$ 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* - $\mathrm{fl}(x)$ 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* - $\mathrm{fl}(x)$ is the nearest normalized floating-point number between $x$ and 0.

*Remark.* A more precise definition of the fl functions exists for even $\beta$. 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 $\mathrm{fl}(x)$ for an $m$-digit floating-point representation with a maximum $M$ exponent is

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

## 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 $\mathrm{fl}(x)$ as an approximation to $x$. Usually it is absolute error $x - \mathrm{fl}(x)$.

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

(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 $\beta, m$ 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 $\delta$ where $\delta \leq u$ where $x, y$ are floating-point numbers. Alternatively,

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

for some $\varepsilon$ 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 $\delta$ 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 $\beta$,

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

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

**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 $\alpha$. The expansion of $N$ in base $\beta$ can be found using two different methods:

(i) Express $\alpha, a_0, a_1, \cdots, a_n$ in base $\beta$. 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 $\beta$ 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 $\alpha$. The expansion of $x$ in base $\beta$ can be found using two different methods:

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

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

where each operation is in base $\beta$ 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 $\beta$. 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): $n(n-1) + \sum_{k=1}^{(n-1)}\left[(n-k+1)+(n-k)\right] \approx 2n^2$,
(iii) scaled pivoting (updating scale factors): $\sum_{k=1}^{(n-1)}\left[(n-k+1)(n-k)+(n-k+1)+(n-k)\right] \approx n^3/3$,
(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,

$$U = (M_{n-1}P_{n-1}) \cdots (M_1P_1)A,$$

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 $P_kM_l = \widetilde{M_l}P_k$ 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.

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

**Definition 2.17.** 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 2.18.** 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 2.19.** 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 2.20.** For $p = 1$ and $p = \infty$, there are explicit expressions for $||A||_1$ and $||A_\infty||$.

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

**Definition 2.21.** Let $\mathbf{x}$ and $\mathbf{y}$ be vectors in $\mathbb{R}^n$ where $\mathbf{x} = (x_1, x_2, \ldots, x_n)^\top$ and $\mathbf{y} = (y_1, y_2, \ldots, y_n)^\top$. We recall the familiar *scalar product*, or dot product given by

$$\mathbf{x}^\top \mathbf{y} = x_1 y_1 + x_2 y_2 + \cdots + x_n y_n.$$

**Lemma 2.22.** For all vectors $\mathbf{x}$, $\mathbf{y}$, and $\mathbf{z}$ in $\mathbb{R}^n$ and for all scalars $\alpha$:

(i) $\mathbf{x}^\top \mathbf{y} = \mathbf{y}^\top \mathbf{x}$,

(ii) $(\alpha \mathbf{x})^\top \mathbf{y} = \alpha(\mathbf{x}^\top y)$,

(iii) $(\mathbf{x} + \mathbf{y})^\top \mathbf{z} = \mathbf{x}^\top z + \mathbf{y}^\top z$,

(iv) $\mathbf{x}^\top \mathbf{x} \geq 0$ where $\mathbf{x}^\top \mathbf{x} = 0$ if and only if $\mathbf{x} = 0$

**Theorem 2.23 (The Cauchy-Schwarz Inequality).** Given any $\mathbf{x}$ and $\mathbf{y}$ in $\mathbb{R}^n$, $|\mathbf{x}^\top \mathbf{y}| \leq ||\mathbf{x}||_2 ||\mathbf{y}||_2$.

**Theorem 2.24.** The operator norm $||A||_2$ is the square root of the largest eigenvalue of $A^H A$.

**Definition 2.25.** 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 $\mathbf{x} \in \mathcal{F}^n$, $||A\mathbf{x}||_v \leq ||A||_m \cdot ||\mathbf{x}||_v$.

**Definition 2.26.** 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 2.27.** The Frobenius norm of $A$ is compatible with $||\mathbf{x}||_2$.

## 2.5 Residual Error

**Definition 2.28.** 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 2.29.** For all $n$-vector $\mathbf{y}$ for an invertible matrix $A$ such that $A\mathbf{x} = \mathbf{b}$,

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

**Definition 2.30.** Define $\kappa(A) = ||A|| \cdot ||A^{-1}||$ to be the *condition number of* $A$ when $\kappa(A) \geq 1$.

**Theorem 2.31.** 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 2.32.** 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 2.33.** In general, the bound on the error in $\hat{\mathbf{x}}$ relative to $\hat{\mathbf{x}}$ is

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

**Theorem 2.34.** 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.

## 2.6 General Iterative Methods

**Definition 2.35 (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 2.36.** 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 2.37.** 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 2.38 (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 2.39.** 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 2.40 (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:

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

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

**Definition 2.41.** A matrix is called *(strictly row) diagonally dominant* if

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

**Theorem 2.42.** If $A$ is diagonally dominant, then Jacobi's Method converges.

**Definition 2.43 (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 $k$th iteration (computing $\mathbf{x}^{(k+1)}$ from $\mathbf{x}^{(k)}$), this system for $\mathbf{x}^{(k+1)}$ is solved by forward substitution.

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

for $1 \le i \le n$ 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 2.44.** 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 2.45.** 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 $\mathbf{x} \ne \mathbf{0}$, $\mathbf{x}^\top A\mathbf{x} > 0$.

**Theorem 2.46.** A real symmetric $n \times n$ matrix is positive definite if and only if all of its eigenvalues are positive.

**Theorem 2.47.** 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 2.48 (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 $\omega$ 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,

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

## 2.7 Linear Least Squares

**Definition 2.49 (Linear Least Squares).** Often times the linear system $A\mathbf{x} = \mathbf{b}$ where $A$ is an $m \times n$ real matrix and $\mathbf{b} \in \mathbb{R}^m$ has no solution since $m > n$. The range of $A$ has dimension less than or equal to $n < m$ so it is a proper subspace of $\mathbb{R}^m$ and there are many $\mathbf{b} \in \mathbb{R}^m$ for which no solution exists. Instead, we find a vector $\mathbf{x} \in \mathbb{R}^n$ that minimizes

$$||\mathbf{e}||_2^2 = ||A\mathbf{x} - \mathbf{b}||_2^2 = \sum_{i=1}^{m} \left( \sum_{j=1}^{n} a_{ij} x_j - b_i \right)^2,$$

the sum of the squares of the error terms.

**Theorem 2.50.** Let $Y$ be a subspace of $\mathbb{R}^m$ and let $\mathbf{b} \in \mathbb{R}^m$. Then there is a unqiue closest element $\hat{\mathbf{y}}$ of $Y$ to $\mathbf{b}$ in the 2-norm $||\cdot||_2$, i.e. $||\mathbf{b} - \hat{\mathbf{y}}||_2 \leq ||\mathbf{b} - \mathbf{y}||_2$ for all $\mathbf{y} \in Y$ and $||\mathbf{b} - \hat{\mathbf{y}}||_2 < ||\mathbf{b} - \mathbf{y}||_2$ for $y \neq \hat{\mathbf{y}}$. Moreover, $\mathbf{b} - \hat{\mathbf{y}}$ is orthogonal to $Y$ i.e. $(\mathbf{b} - \hat{\mathbf{y}})^\top \mathbf{y} = 0$ for all $\mathbf{y} \in Y$.

**Theorem 2.51 (The Normal Equations).** Given a real $m \times n$ matrix $A$, vectors $\mathbf{a}, \mathbf{b} \in \mathbb{R}^m$ and $\mathbf{x} \in \mathbb{R}^n$ minimizes $||A\mathbf{x} - \mathbf{b}||_2^2$ if and only if $\mathbf{x}$ is a solution of the normal equations

$$A^\top A\mathbf{x} = A^\top \mathbf{b}.$$

*Remark.* Computation concerns with linear least squares:

(i) The normal equations are often very ill-conditioned in the 2-norm, $\kappa(A^\top A) = \kappa(A)^2$, so it is not always best to use the normal equations.

(ii) Better numerical methods for linear least squares problems: QR factorization (closely related to Gram-Schmidt), Singular Value Decomposition (for ill-conditioned problems).

# 3 Solutions of Non-Linear Systems

## 3.1 Methods for Solving Non-Linear Systems

**Definition 3.1.** A real number $x$ for which $f(x) = 0$ is called a *root* of that equation; $x$ is called a *emph* of $f$.

**Definition 3.2 (General Methods of Solving Linear Equations).** To solve a non-linear equation, write it in the form $f(x) = 0$, assuming that $f$ is a continuous real-valued function that is defined on some interval $I \in \mathbb{R}$. In practice, locate approximately a zero $s$ of the given function $f$. We want to find an $x$ such that $|x - s|$ is small or $|f(x)|$ is small.

**Theorem 3.3.** If $f$ is continuous on $[a, b]$ and $f(a)f(b) < 0$, then there exists an $s \in (a, b)$ for which $f(s) = 0$.

**Definition 3.4 (Bisection Method).** The *bisection method* is a bracketing method where at each step in the iteration, we have an interval $[a, b]$ in which $f$ as a 0. Start with an interval $[a, b]$ that brackets a zero of $f$, i.e. $f(a)f(b) < 0$. For each step, shrink the length of the interval by a fator of 2 while still bracketing a zero of $f$. The bisection method is guaranteed to converge, but it has a slow convergence rate, approximately 3 iterations per decimal digit of accuracy.

**Definition 3.5 (Newton's Method).** Start with an approximation $x_0$ to $s$. Iteratively, find the zero of the tangent line to the graph of $f$ at $(x_n, f(x_n))$ to get $x_{n+1}$. Converges rapidly if it converges, so it needs to start sufficiently close to the zero and we ened to be able to evaluate $f'$, i.e. computable and $f'(s) \neq 0$.

**Definition 3.6 (Secant Method).** Start with two approximations $x_{n-1}$ and $x_n$ to $s$. Find the zero of the secant line joining the two previous points $(x_{n-1}, f(x_{n-1}))$, $(x_n, f(x_n))$. Similar to Newton's method with a slower convergence, but $f'$ is not required to evaluate the derivative $f'$.

*Remark.* Ideally, we would like the dependability of the bisection method and the speed of Newton. For example, *Regular Falsi* (see text) is a bracketing method similar to the secant method. Often, one endpoint converges quickly to a zero of $f$. *Brent's Method* (also called the *Brent-Dekker method*) is a combination of bisection, secant, and inverse quadratic interpolation that converges rapidly.

## 3.2 Fixed-Point Iteration

*Remark.* Many iterative methods, e.g. Newton's method, can be viewed as $x_{n+1} = g(x_n)$ where $g$ is some particular function.

**Definition 3.7.** For a function $g$, a *fixed point* of $g$ is a point $x$ where $g(x) = x$.

**Theorem 3.8.** If $x_{n+1} = g(x_n)$ where $g$ is continuous and $x_n$ converges to a number $\zeta$ in the domain of $g$, then $g(\zeta) = \zeta$, i.e. $\zeta$ is a fixed point.

**Theorem 3.9.** Let $g$ be a continuous function on a closed bounded interval $I = [a, b]$, and suppose for all $x \in I$, $g(I) \in I$, i.e. $g$ maps $I$ to itself. Then $g$ has at least one fixed point in $I$.

**Theorem 3.10 (Contraction Mapping Fixed-Point Theorem, Differentiable Functions).** Suppose $g$ is differentiable on a closed, bounded interval $I = [a, b]$, that $g$ maps $I$ to itself, and for some $L < 1$, $|g'(x)| \leq L < 1$ for all $x \in I$. Then the following are true:

(i) $g$ has a unique fixed point in $I$; call it $\zeta$,

(ii) if for any $x_0 \in I$, $x_{n+1} = g(x_n)$ generates a sequence such that $x_n \to \zeta$,

(iii) if $e_n = x_n - \zeta$, then

$$|e_n| \leq \frac{L^n}{1-L}|x_1 - x_0|.$$

**Corollary 3.11 (Local Convergence Theorem).** Suppose $g$ is continuously differentiable in an open interval $I$ containing a fixed point $\zeta$, and suppose $|g'(\zeta)| < 1$. Then there exists an $\epsilon > 0$, so that when $|x_0 - \zeta| \leq \epsilon$, the fixed-point iteration $x_{n+1} = g(x_n)$ yields a sequence $x_n$ with $x_n \to \zeta$.

**Definition 3.12.** Let $x_0, x_1, x_2, \dots$ be a sequence which converges to a number $\zeta$. Let $e_n = x_n - \zeta$. If there is a number $p \geq 1$ and a constant $C \neq 0$ for which

$$\lim_{n\to\infty} \frac{|e_{n+1}|}{|e_n|^p} = C$$

then $p$ is called the *order of convergence* of the sequence and $C$ is called the *asymptotic error constant*.

**Definition 3.13.** For specific values of $p$ and $C$ we assign specific names to the order of convergence:

(i) if $p = 1$ and $C = 1$, convergence is called *sub-linear*;

(ii) if $p = 1$ and $0 < C < 1$, convergence is called *linear*;

(iii) if $\lim_{n\to\infty} |e_{n+1}|/|e_n| = 0$, convergence is called *super-linear*;

(iv) if $p = 2$, convergence is called *quadratic*.

**Definition 3.14.** A function $f \in C^k$ on an interval $[a, b]$ where $k$ is a non-negative integer when $f, f', f'', \dots, f^{(k)}$ are all defined and continuous on $[a, b]$. In the case of $k = 0$, $f$ is continuous. In the case of $k = 1$, $f$ is continuously differentiable.

**Theorem 3.15 (Taylor's Theorem with Remainder).** If $f \in C^{k+1}$ then for each $x$, there exists a $\zeta$ between $a$ and $x$ for which

$$f(x) = f(a) + f'(a)(x-a) + \cdots + \frac{f^{(k)}(a)}{k!}(x-a)^k + \frac{f^{(k+1)}(\zeta)}{(k+1)!}(x-a)^{k+1}.$$

**Theorem 3.16.** Suppose $g \in C^{k+1}$, $g(s) = s$, $x_n$ is generated by $x_{n+1} = g(x_n)$ and $x_n \to s$, and $g'(s) = g''(s) = \cdots = g^{(k)}(s) = 0$ and $g^{(k+1)}(s) \neq 0$. Then $x_n \to s$ to order $k+1$ with an asymptotic error constant of $|g^{(k+1)}(s)|/(k+1)!$.

**Theorem 3.17.** Suppose $f \in C^3$, $f(s) = 0$, $f'(s) \neq 0$, and $x_n$ is generated by Newton's method $x_{n+1} = x_n - f(x_n)/f'(x_n)$. Then

(i) if $x_n \to s$, convergence is at least quadratic,

(ii) if $x_0$ is close enough to $s$, then $x_n \to s$.