Iterative method

Convergence criterion:

Theorem: Let A be a square matrix. Then

$$\lim_{k\to\infty} A^k x = 0 \text{ for every } x \in \mathbb{R}^n$$

is equivalent to,

$$\rho(A) < 1$$

where $\rho(A)$ is the spectral radius.

Iterative method

Convergence criterion:

Theorem: The sequence $\{x^k\}_{k=0}^{\infty}$ that is defined by

$$x^{k+1} = Tx^k + c, \quad \forall k \geq 0$$

converges to the solution of

$$x = Tx + c$$

if and only if $\rho(T) < 1$.

This is known as fixed point iteration.

Iterative method

Proof: Let $\rho(T) < 1$.

$$\begin{aligned} x^{k+1} &= Tx^k + c \\ &= T(Tx^{k-1} + c) + c \\ &= \ldots\ldots \\ &= T^{k+1}x^0 + (T^k + \cdots + M + I)c \\ &= T^{k+1}x^0 + \sum_{j=0}^{k} T^k c \\ \lim_{k\to\infty} x^k &= \lim_{k\to\infty} T^{k+1}x^0 + \sum_{j=0}^{\infty} T^k c \end{aligned}$$

Iterative method

Since $\rho(T) < 1$, then $\lim_{k\to\infty} T^k x^0 = 0$ for every x^0 and

$$\sum_{j=0}^{\infty} T^k = (I - T)^{-1}.$$

Therefore

$$\lim_{k\to\infty} x^k = (I - M^{-1})c = x.$$

This implies that

$$x = Tx + c.$$

To prove the converse, let z be an arbitrary, and x be the unique solution to $x = Tx + c$.

Iterative method

Let $x^{k+1} = Tx^k + c$ for $k \geq 0$ and the sequence $\{x^k\}_{k=0}^{\infty}$ converge to x. Define $x^0 = x - z$.

$$
\begin{aligned}
x - x^k &= Tx + c - (Tx^{k-1} + c) \\
&= T(x - x^{k-1}) \\
&= T(T(x - x^{k-2})) \\
&= \vdots \\
&= T^k(x - x^0) \\
&= T^k z \\
\lim_{k \to 0} T^k z &= \lim_{k \to 0} (x - x^k) = 0
\end{aligned}
$$

Since this is true for any $z \in \mathbb{R}^n$, we must have $\rho(T) < 1$

Direct method

Problem:

Find the number of arithmetic operations for forward Gauss elimination process.

Solution: At i-th column, $n-i$ division is required to reduce all elements below the diagonal.

The total # of divisions is $\sum_{i=1}^{n-1}(n-i) = n^2/2 - n/2$.

Direct method

Ignoring leading zero elements, $n-i+1$ multiplications are required at $n-i$ rows of the augmented matrix.

The total # of multiplications are

$$\sum_{i=1}^{n-1}(n-i+1)(n-i) = n^3/3 - n/3.$$

The # of subtractions are same as that of multiplications.

The total # of operations is $2n^3/3 + n^2/2 - 7n/6 = \mathcal{O}(n^3)$.

Direct method

Problem:

Find the number of arithmetic operations for back substitution in Gauss elimination process.

Solution:

At i-th row, $n-i$ multiplications are required.

Such multiplications are required at $(n-1)$ rows (except the last one).

The total # of multiplications: $\sum_{i=1}^{n-1} i = n^2/2 - n/2$

Direct method

The total # of divisions: n.

The # of subtraction is same as the number of multiplications.

The total # of operations for back substitution is n^2.

Exercise: Determine the computational complexity of the Gauss elimination process.

Direct method

Sparse matrix:

A square matrix $A = [a_{ij}]$ is said to be tridiagonal if

$$a_{ij} = 0$$

for all pairs (i, j) that satisfies $|i - j| > 1$.

Direct method

Sparse matrix:

A tri-diagonal system may be written as:

$$
\begin{aligned}
d_1 x_1 + c_1 x_2 &= b_1 \\
a_i x_{i-1} + d_i x_i + c_i x_{i+1} &= b_i; \quad 2 \leq i \leq n-1 \\
a_n x_{n-1} + d_n x_n &= b_n
\end{aligned}
$$

The coefficient matrix A has all elements zero other than 3 main diagonal elements.

Direct method

Sparse matrix:

The tri-diagonal matrix is:

$$A = \begin{bmatrix} d_1 & c_1 & 0 & 0 & 0 & 0 & 0 \\ a_2 & d_2 & c_2 & 0 & 0 & 0 & 0 \\ 0 & a_3 & d_3 & c_3 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & a_n & d_n \end{bmatrix}$$

Therefore, it is not necessary to store and calculate all elements.

Considering this fact, we can reduce the cost of direct solver.

Direct method

Thomas algorithm:

Let $A = LU$ be the LU decomposition of the tri-diagonal matrix A, where

$$L = \begin{bmatrix} 1 & & & & & \\ l_{21} & 1 & & & & \\ & l_{32} & 1 & & & \\ & & & & & \\ & & & & & \\ & & & l_{n-1,n} & 1 & \end{bmatrix}$$

$$U = \begin{bmatrix} u_{11} & u_{12} & & & & \\ & u_{22} & u_{23} & & & \\ & & u33 & u_{34} & & \\ & & & & & \\ & & & & u_{nn} & \end{bmatrix}$$

Direct method

LU decomposition of tri-diagonal system

i-th row of L × i-th column of U

$$l_{i\,i-1}\,u_{i-1\,i} + u_{ii} = a_{ii} = \boxed{d_i}, \quad i = 2, \cdots n$$

(i-1)-th row of L × i-th columns of U

$$u_{i-1\,i} = a_{i-1\,i} = \boxed{c_{i-1}}, \quad i = 2, 3, \cdots n$$

i-th row of L × (i-1)-th column of U

$$l_{i\,i-1}\,u_{i-1\,i-1} = a_{i\,i-1} = \boxed{a_i} \quad i = 2, 3, \cdots n$$

Thus.

$$u_{11} = a_{11} = \boxed{d_1}$$

$$\left.\begin{aligned} l_{i\,i-1} &= \frac{a_{i\,i-1}}{u_{i-1\,i-1}} \\ u_{ii} &= a_{ii} - l_{i\,i-1}\,u_{i-1\,i} \\ &= a_{ii} - l_{i\,i-1}\,a_{i-1\,i} \end{aligned}\right\} \quad i = 2, 3, \cdots n$$

Direct method

Thomas algorithm:

The elements l_{ij} and u_{ij} are determined as

$$\begin{aligned} u_{11} &= a_{11} \\ l_{i,i-1} &= \frac{a_{i,i-1}}{u_{i-1,i-1}} \\ u_{ii} &= a_{ii} - l_{i,i-1}a_{i-1,i}, \;\; i = 2, 3, \ldots, n \end{aligned}$$

Direct method

The solution of $A\mathbf{x} = \mathbf{b}$ is computed using:

Forward

$$\begin{aligned} z_1 &= b_1 \\ z_i &= b_i - l_{i,i-1} z_{i-1}, \quad i = 2, 3, \ldots, n \end{aligned}$$

Backward

$$\begin{aligned} x_n &= \frac{z_n}{u_{nn}} \\ x_i &= \frac{z_i - a_{i,i+1} x_{i+1}}{u_{ii}}, \quad i = n-1, n-2, \ldots, 1. \end{aligned}$$

The above algorithm is known as Thomas algorithm.

Solution of nonlinear equations

How does one solve equations

$$f(x) = 0?$$

Example:

$$f(x) := 3x + \sin(x) - e^x = 0.$$

If we plot $f(x)$ for $0 \leq x \leq 1$, we see that $f(0) = -1$, $f(1) = 1.12$, and $f(2) = -0.47$.

Bisection method

Theorem: If $f(x)$ is continuous and changes sign in $[a, b]$, then there is a constant c such that $f(c) = 0$. We call $x = c$ is a zero or root of $f(x) = 0$.

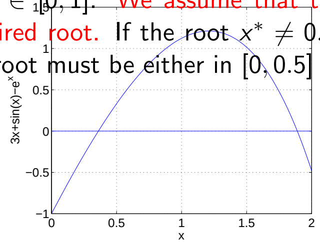
Approximate solution: Let $\epsilon > 0$ and a continuous function $f(x)$ satisfies

$$f(a) \cdot f(b) < 0$$

in a given interval $[a, b]$. We say that $c = (a + b)/2$ is an approximate solution if $|f(c)| \leq \epsilon$.

Bisection method

Want to solve $f(x) := 3x + \sin(x) - e^x = 0$. Since $f(0) \cdot f(1) < 0$, we assume that there is a root $x^* \in [0, 1]$. We assume that the mid-point of the interval is the desired root. If the root $x^* \neq 0.5$, we divide the interval. Clearly, the root must be either in $[0, 0.5]$ or in $[0.5, 1]$.



The procedure will continue until the tolerance

$$|f(x^*)| \leq \epsilon,$$

which implies that x^* is an approximate root.

Bisection method

algorithm:

1. Determine the interval $[a, b]$ by inspection.
2. Let $x = (a + b)/2$ is the solution.
3. Check convergence criterion: If

$$f(x) \leq \epsilon$$

   is satisfied, then stop.
4. If $f(a) \cdot f(x) > 0$, then both $f(a)$ and $f(x)$ have the same sign. Hence, replace a by x and go to step (2)
5. If $f(a) \cdot f(x) < 0$, then $f(a)$ and $f(x)$ have opposite sign. Hence, replace b by x and go to step (2)

Bisection method

Let c_n be the approximation of the true solution x^* after n steps of Bisection method. Prove the following error bound

$$|x^* - c_n| \leq 2^{-n}(b - a).$$

Let $c_{i+1} = (a_i + b_i)/2$ be the approximation at i-th step and the next interval is $[a_{i+1}, b_{i+1}]$, where $a_{i+1} = a_i$ and $b_{i+1} = c_{i+1}$ or $a_{i+1} = c_{i+1}$ and $b_{i+1} = b_i$. Then $b_{i+1} - a_{i+1} = \frac{b_i - a_i}{2}$. If $a_0 = a$ and $b_0 = b$, we can write

$$b_n - a_n = 2^{-n}(b - a)$$

and

$$f(b_n)f(a_n) \leq 0.$$

Bisection method

Clearly,

$$\lim_{n\to\infty}(b_n - a_n) = 0.$$

Let $x^* = \lim_{n\to\infty} b_n = \lim_{n\to\infty} a_n$.

We get $\lim_{n\to\infty} f(a_n)f(b_n) \leq 0$ implies $[f(x^*)]^2 \leq 0$. Therefore, $f(x^*) = 0$.

The error bound at n-th step is

$$|x^* - c_n| \leq 2^{-n}|b - a|$$

since $a_{n-1} \leq x^* \leq c_n \leq b_{n-1}$ or $a_{n-1} \leq c_n \leq x^* \leq b_{n-1}$.

Bisection method

Example: Solve $3x + sin(x) - e^x = 0$ in the interval $[0, 1]$ using a tolerance 10^{-1}.

Solution: Let $a = 0$, and $b = 1$. Then $f(a) = -1$ and $f(b) = 1.1232$.

Let $x = (a + b)/2 = 0.5$. Then $f(x) = 0.3307$. Since $f(a) \cdot f(x) < 0$, we set $b = 0.5$ and $x = (a + b)/2 = 0.25$.

Now $f(x) = -0.2866$ and $f(x) \cdot f(b) < 0$. So we set $a = 0.25$ and $x = (a + b)/2 = 0.3750$. We get $f(x) = 0.0363$.

Since $|f(x)| < 10^{-1}$, the desired solution is $x^* = 0.375$.

Secant method

Let x^* be such that $f(x^*) = 0$.

Suppose that x_0 and x_1 are two points such that $|f(x_1)| < |f(x_0)|$. Then $|x^* - x_1| < |x^* - x_0|$.

Let the straight line joining points $(x_0, f(x_0))$ and $(x_1, f(x_1))$ passes through the point $(x_2, 0)$.

Using similar triangles,

$$\frac{x_1 - x_2}{f(x_1)} = \frac{x_0 - x_1}{f(x_0) - f(x_1)}.$$

Secant method

Using similar triangles,

$$\frac{x_1 - x_2}{f(x_1)} = \frac{x_0 - x_1}{f(x_0) - f(x_1)}.$$

Therefore,

$$x_2 = x_1 - f(x_1)\frac{x_0 - x_1}{f(x_0) - f(x_1)}.$$

Repeating the procedure, we get:

$$x_{n+1} = x_n - f(x_n)\frac{x_{n-1} - x_n}{f(x_{n-1}) - f(x_n)}.$$