Numerical Analysis

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1 Numerical Linear Algebra

1.1 Linear System of Equations

The simplest problem we can consider in linear algebra is to solve an equation that's in the form

$$A\mathbf{x} = \mathbf{b}, \tag{1}$$

where $A \in \mathbb{R}^{n \times n}$, and $\mathbf{x}, \mathbf{b} \in \mathbb{R}^n$.

Trivially, we know how the solve such a problem in general, to find the inverse of A (if A is not singular). But this is inefficient and requires heavy computing power, so we will seek better algorithms for solving such problems.

1.1.1 Triangular Matrices

Triangular matrices are nicer to work with than general matrices. One example of this is that the determinant of a triangular matrix is just the product of its diagonal, i.e. given an triangular matrix $A \in \mathbb{R}^{n \times n}$ (no matter upper of lower triangular),

$$\det A = \prod_{i=1}^{n} A_{i,i}.$$

Immediately, we can deduce that an triangular matrix is non-singular if and only if it has no zero entries in its diagonal.

Let us consider equation 1 where A is an upper triangular matrix.

$$\begin{bmatrix} A_{1,1} & A_{1,2} & \cdots & A_{1,n} \\ 0 & A_{2,2} & \cdots & A_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & A_{n,n} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}. \tag{2}$$

We can immediately see that $x_n = b_n / A_{n,n}$, and $x_{n-1} = (b_{n-1} - A_{n-1,n} x_n)/A_{n-1,n-1}$. Indeed,

$$x_i = \frac{1}{A_{i,i}} \left(b_i - \sum_{j=1+i}^{n} A_{i,j} x_j \right),$$

and similarly, for A, a lower triangular matrix,

$$x_i = \frac{1}{A_{i,i}} \left(b_i - \sum_{j=1}^{i-1} A_{i,j} x_j \right).$$

This method can be used to find the inverse of matrices by considering $A\mathbf{x} = e_k$ gives us the k-th column of A^{-1}. By considering that to calculate each x_i, there is $i-1$ steps, we find that to calculate $\mathbf{x} \in \mathbb{R}^n$, there is $(n^2 - n)/2$ steps, so a complexity of $O(n^2)$.

1.1.2 LU Factorisation

Let $A \in \mathbb{R}^{n\times n}$ (not necessarily triangular), $\mathbf{x}, \mathbf{b} \in \mathbb{R}^n$ such that equation 1 is satisfied. If we can find lower and upper triangular matrices L, U such that $A = LU$, then

$$A\mathbf{x} = LU\mathbf{x} = \mathbf{b},$$

which is easily solvable using the previous algorithm.

However, such an Factorisation is not unique, so we impose the restriction that L is unit, that is to say the diagonals of L are all ones.

Suppose $A = LU$ where

$$L = \begin{bmatrix} \mathbf{l}_1 & \mathbf{l}_2 & \cdots & \mathbf{l}_n \end{bmatrix}, \quad U = \begin{bmatrix} \mathbf{u}_1^T \\ \mathbf{u}_2^T \\ \vdots \\ \mathbf{u}_n^T \end{bmatrix},$$

so $A = \sum_{i=1}^n \mathbf{l}_i \mathbf{u}_i^T$, where $\mathbf{l}_i \mathbf{u}_i^T = \begin{bmatrix} (\mathbf{l}_i)_1 \mathbf{u}_i^T & (\mathbf{l}_i)_2 \mathbf{u}_i^T & \cdots & (\mathbf{l}_i)_n \mathbf{u}_i^T \end{bmatrix}^T$. As L is unit, $(\mathbf{l}_1)_1 = 1$, and as for all $j > 1$, $(\mathbf{l}_j)_1 = 0$ (since L is lower triangular), the first row of A is $\sum_{i=1}^n (\mathbf{l}_i)_1 \mathbf{u}_i^T = 1 \times \mathbf{u}_1^T + 0 \times \mathbf{u}_2^T + \cdots + 0 \times \mathbf{u}_n^T = \mathbf{u}_1^T$. Similarly, by considering the first column of A equals $(\mathbf{u}_1^T)_1 \times \mathbf{l}_1$, we can find $\mathbf{l}_1$.

In general, we find the following algorithm for finding the LU factorisation,

$$\begin{aligned} U_{k,j} &= A_{k,j}^{k-1} \\ L_{i,k} &= A_{i,k}/A_{k,k} \\ A_{i,j}^k &= A_{i,j}^{k-1} - L_{i,k} U_{k,j} \end{aligned}$$

for $k \in \{1, \cdots, n\}$ and $i, j \geq k$ with $A^0 = A$. From this, we can easily see the algorithm breaks down whenever there is some k such that $A_{k,k} = 0$.

Definition 1.1. (Positive definite matrix). A matrix $A \in \mathbb{R}^{n\times n}$ is *positive-definite* if and only if

$$\mathbf{x}^T A \mathbf{x} > 0$$

for $\mathbb{R}^n \ni \mathbf{x} \neq \mathbf{0}$.

Theorem 1. *Given a positive definite matrix $A \in \mathbb{R}^{n\times n}$, its upper left $k \times k$ sub-matrix is non-singular, i.e.*

$$\det(A_k) \neq 0$$

for all $k \in \{1, \cdots, n\}$.

Proof. Let $k \in 1, \cdots, n$ and $\mathbf{x} \in \mathbb{R}^k$ such that $A_k\mathbf{x} = 0$. Now, as A_k is singular if and only if $A_k\mathbf{x} = 0 \implies \mathbf{x} = 0$, it suffices to prove $\mathbf{x} = 0$. We can construct $\mathbf{y} \in \mathbb{R}^n$ by letting $\mathbf{y}_i = \mathbf{x}_i$ for $i \in \{1, \cdots, k\}$ and $\mathbf{y}_i = 0$ for $i \in \{k+1, \cdots, n\}$ so $A\mathbf{y} = 0$ and thus $\mathbf{y}^T A\mathbf{y} = 0$. But A is positive definite, so $\mathbf{y} = \mathbf{0}$ and hence $\mathbf{x} = \mathbf{0}$. $\square$

Theorem 2. *A symmetric matrix $A \in \mathbb{R}^{n\times n}$ is positive definite if and only if*

$$A = LDL^T$$

for some $L, D \in \mathbb{R}^{n\times n}$ where L is unit lower triangular and D diagonal with $D_{k,k} > 0$ for all k.