Notes on Solving Linear Systems

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Many engineering, operation research, and machine learning problems involves solving linear systems of equations. That is, given a non-singular matrix $A \in \mathbb{R}^{m\times m}$, and a vector $b \in \mathbb{R}^m$, solve the following equation for $x \in \mathbb{R}^m$:

$$Ax = b \tag{1}$$

Finite-element method to solve differential equations, maximum likelihood estimation or ordinary least squares where some of the optimal solution forms of parameter estimations can be reduced to a linear system are typical examples. This tutorial are based on two textbooks [1], [2], and will only go over the most general technique, and the special case when A is symmetric and positive definite. Other augmented or related topics such as, LU factorization with partial pivoting, preconditioning, or iterative methods might be covered in the future and are temporally leaved for readers to explore upon their interest.

1 LU Factorization

1.1 An Illustrative Case

Consider the following 2-by-2 linear system:

$$\begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} x = \begin{bmatrix} 1 \\ 1 \end{bmatrix} \tag{2}$$

The most straightforward way you might know to solve the system is by Gaussian eliminations. To do it, you can construct your augmented matrix $[A|\ b]$, multiply the first row by 3, and subtract it from the second row. This will give you:

$$\left[\begin{array}{cc|c} 1 & 2 & 1 \\ 0 & -2 & -2 \end{array}\right] \tag{3}$$

To continue the elimination, we can simply add the new second row back to the first row:

$$\left[\begin{array}{cc|c} 1 & 0 & -1 \\ 0 & -2 & -2 \end{array}\right] \tag{4}$$

which implies the solution is $x = \begin{bmatrix} -1 \\ 1 \end{bmatrix}$.

The two steps of Gaussian eliminations respectively introduce a 0 to the lower left and upper right elements on A. Let us see these processes on the original matrix A again but in matrix operation. The first operation is equivalent to a matrix-matrix product:

$$\begin{bmatrix} 1 & 2 \\ 0 & -2 \end{bmatrix} = \hat{L} \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix} \tag{5}$$

where

$$\hat{L} = \begin{bmatrix} 1 & 0 \\ -3 & 1 \end{bmatrix} \tag{6}$$

Note that the inverse of $\hat{L}$ is just the same martix with an opposite sign on the lower left term:

$$L = \hat{L}^{-1} = \begin{bmatrix} 1 & 0 \\ 3 & 1 \end{bmatrix} \tag{7}$$

so we can multiply L on the left, and let $U = \begin{bmatrix} 1 & 2 \\ 0 & -2 \end{bmatrix}$, A is the product of LU:

$$A = LU = \begin{bmatrix} 1 & 0 \\ 3 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 0 & -2 \end{bmatrix} \tag{8}$$

where L is a lower triangular matrix and U is an upper triangular matrix. We should see the benefit of doing this decomposition soon. Now, with the L and U matrices, we can split the problem of solving $Ax = b$ into two triangular systems. That is, let $y = Ux$, we first solve:

$$Ly = b \tag{9}$$

for y, and then solve:

$$Ux = y \tag{10}$$

for x. Solving triangular systems are much easier to do. The system $Ly = b$ already tells us $y_1 = 1$ by looking at the first row (the second term of the first row is 0). We just need to put $y_1 = 1$ into the second equation and solve for y_2, and we get $y_2 = -2$. Note that the solution y is just the last column of the augmented matrix $[A|\ b]$ after applying the first step of the Gaussian elimination above. Then we turn to solve $Ux = y$. The last row of U already informs that $x_2 = 1$ since the first element of the last row is 0. By putting $x_2 = 1$ into the first row's equation, we have $x_1 = -1$. Note that solving the second triangular system is equivalent to the second step of the previous Gaussian eliminations.

1.2 LU Decomposition in General

The above case study suggests a powerful method to solve any general linear system, $Ax = b$. We can compute the LU factorization of A, and then solve two triangular systems using backward substitution and forward substitution since solving them are equivalent to an implementation of Gaussian eliminations. We first show the theorem of the existence of LU factorization.

Theorem. *Let $A \in \mathbb{R}^{m\times m}$, there exists $U,\ L \in \mathbb{R}^m$ such that U is an upper triangular matrix, and L is lower triangular such that $A = LU$.*

Proof. Let us use $A_{i,j}$ for $i, j = 1, 2, 3 \cdots m$ to denote elements on A matrix. Assume that $A_{j,j} \neq 0$ for $j = 1, 2 \cdots m$, choose $\hat{L}_k$ as:

$$\hat{L}_k = \begin{bmatrix} 1 & 0 & & \cdots & 0 & 0 \\ 0 & 1 & & \cdots & 0 & 0 \\ 0 & 0 & 1 & & 0 & 0 \\ \vdots & \vdots & -\ell_{k+1,k} & \ddots & \vdots & \vdots \\ 0 & 0 & -\ell_{k+2,k} & 1 & 0 & 0 \\ 0 & 0 & \vdots & 0 & 1 & 0 \\ 0 & 0 & -\ell_{m,k} & 0 & 0 & 1 \end{bmatrix}$$

where $\ell_{j,k} = \frac{A_{j,k}}{A_{k,k}}$ for $j = k+1, k+2 \cdots m$. Multiply $\hat{L}_k$ to the left hand side of A will make every elements of the k column of A below the diagonal become 0. Moreover, for any k_1 and k_2 with $k_1 \neq k_2$:

$$\hat{L}_{k_1}\hat{L}_{k_2} = \begin{bmatrix} 1 & 0 & & \cdots & 0 & 0 \\ 0 & 1 & & \cdots & 0 & 0 \\ 0 & 0 & 1 & & 0 & 0 \\ \vdots & \vdots & -\ell_{k_1+1,k_1} & 1 & \vdots & \vdots \\ 0 & 0 & -\ell_{k_1+2,k_1} & -\ell_{k_2+1,k_2} & & 0 \\ 0 & 0 & \vdots & \vdots & 1 & 0 \\ 0 & 0 & -\ell_{m,k_1} & -\ell_{m,k_2} & 0 & 1 \end{bmatrix}$$

which also a lower triangular matrix.
Therefore, consider multiply $\hat{L}_1$, $\hat{L}_2$, ... $\hat{L}_{m-1}$ consecutively:

$$\hat{L}_{m-1}\hat{L}_{m-2}\cdots\hat{L}_1 A$$

is an upper triangular matrix, and $L = \left(\hat{L}_{m-1}\hat{L}_{m-2}\cdots\hat{L}_1\right)^{-1}$ is lower triangular because the inverse of an lower triangular matrix is also lower triangular. $\square$

Remember that for each $\hat{L}k$, the inverse of it is:

$$\hat{L}_k^{-1} = \begin{bmatrix} 1 & 0 & & \cdots & 0 & 0 \\ 0 & 1 & & \cdots & 0 & 0 \\ 0 & 0 & 1 & & 0 & 0 \\ \vdots & \vdots & \ell_{k+1,k} & \ddots & \vdots & \vdots \\ 0 & 0 & \ell_{k+2,k} & 1 & 0 & 0 \\ 0 & 0 & \vdots & 0 & 1 & 0 \\ 0 & 0 & \ell_{m,k} & 0 & 0 & 1 \end{bmatrix} \tag{11}$$

1.3 Backward(Forward) Substitution

We should break down the computation steps for the readers to solve any lower(upper) triangular systems. First, let $Lx = b$ be any lower triangular system. The computation of each x_i for $i = 1, 2 \cdots m$ is:

$$x_i = \frac{b_i - \sum_{j=1}^{i-1} L_{j,i} x_j}{L_{i,i}} \tag{12}$$

which is called forward substitutions.
Similarly, for an upper triangular system $Ux = b$, for any $i = m, m-1 \cdots 2, 1$:

$$x_i = \frac{b_i - \sum_{j=1}^{i-1} U_{i,j} x_j}{U_{i,i}} \tag{13}$$

which is called backward substitutions. Note that the indexing must be in reverse order, i.e. $i = m, m-1 \cdots 2, 1$.

1.4 Cholesky Factorization

The LU factorization has a special case when A is symmetric positive definite. The definition of symmetric positive definiteness is:

Definition 1. *A symmetric matrix $A \in \mathbb{R}^{m\times m}$ is positive definite if and only if $x^\top Ax > 0$ for any $x \in \mathbb{R}^m$.*

Lemma 1. *A symmetric matrix $A \in \mathbb{R}^{m\times m}$ is positive definite if and only if all of its eigenvalues are strictly positive.*

Proof. To show any "if and only if" claim, we need to show that if given A is true, B is true, and the reverse which means given B, A is also true.

Let us start with assuming A is symmetric positive definite. Then, for any $x \in \mathbb{R}^m$, $x^\top Ax > 0$. Therefore, if λ_i and v_i are an eigenvalue of A and its corresponding eigenvector v_i, $v_i^\top Av_i = \lambda_i v_i^\top v_i = \lambda_i \|v_i\|_2^2 > 0$. Since $v_i \neq 0$, $\lambda_i > 0$.

Then, we show the opposite direction. Given that a symmetric A has strictly positive eigenvalues, by spectral theorem, there exists an eigen-decomposition of A, such that $A = U\Sigma U^\top$, where $\Sigma = \mathrm{diag}(\lambda_1, \lambda_2 \cdots, \lambda_m)$ and U is orthogonal. Let $U^\top x = y$, we have $x^\top Ax = x^\top U\Sigma U^\top x = y^\top \Sigma y = \sum_{i=1}^m y_i^2 \lambda_i > 0$, since λ_i are strictly positive. □

In practice, computing all the eigenvalues can be hard and the best way to check the positive definiteness of any symmetric matrix is by computing the Cholesky factorization. If the algorithm fails, the matrix is not positive definite.

Theorem. *A symmetric and positive definite matrix $A \in \mathbb{R}^{m\times m}$ has a Cholesky factorization such that $A = LL^\top$ where L is a lower triangular matrix.*

Proof. The proof is similar to the LU factorization. Consider A matrix, with an assumption that all the diagonal elements of A are nonzero, such that:

$$A = \begin{bmatrix} A_{1,1} & c_1^\top \\ c_1 & A_{2:m,2:m} \end{bmatrix}$$

where $A_{1,1}$ is the upper top element of A (which is a scalar), c_1 is both the first row and first column of A without the first element, and $A_{2:m,2:m}$ is the sub-matrix of A by removing the first row and the first column from A.

We pick $\hat{L}_1$ to be:

$$\hat{L}_1 = \begin{bmatrix} 1 & 0 \\ -c_1/A_{1,1} & I_{m-1} \end{bmatrix}$$

I_{m-1} is the identity matrix of the size $(m-1)$. If multiply $\hat{L}_1$ to the left and $\hat{L}_1^\top$ to the right of A:

$$\hat{L}_1 A \hat{L}_1^\top = \begin{bmatrix} A_{1,1} & 0 \\ 0 & A_{2:m,2:m} - c_1 c_1^\top / A_{1,1} \end{bmatrix}$$

We should use $\hat{A}_2 = A_{2:m,2:m} - c_1 c_1^\top / A_{1,1}$.

For general case, when $k = 1, 2 \cdots m-1$, we define the matrix $\hat{L}_k$ to be with $c_k = \hat{A}_k(1, 2:m)$:

$$\hat{L}_k = \begin{bmatrix} I_k & 0 \\ -c_k/\hat{A}_k(1,1) & I_{m-k} \end{bmatrix}$$

with $\hat{A}_1 = A$, and $\hat{A}_k(1,1)$ denote the upper left element of $\hat{A}_k$. We need to also prove that each sub-matrix $\hat{A}_k$ is symmetric and positive definite. We use mathematical induction. For $k = 1$, this is trivial. For general k, since $x^\top \hat{A}_k x > 0$, consider $\hat{x}_k$ is an arbitrary vector with the first element equals 0. Therefore, $\hat{x}_k^\top \hat{A}_k \hat{x}_k = x^\top \hat{A}_{k+1} x > 0$.

Let us continue the process through every column:

$$\hat{L}_{m-1}\hat{L}_{m-2}\cdots\hat{L}_1 A \hat{L}_1^\top \cdots \hat{L}_{m-2}^\top \hat{L}_{m-1}^\top = \mathcal{D}$$

where $\mathcal{D}$ is a diagonal matrix. Define $L = \left(\hat{L}_{m-1}\hat{L}_{m-2}\cdots\hat{L}_1\right)^{-1}$, we have:

$$A = L\mathcal{D}L^\top = L\sqrt{\mathcal{D}}\sqrt{\mathcal{D}}L^\top$$

with the square root well-defined because every $\hat{A}_k$ is symmetric positive definite so each top left element of $\hat{A}_k$ is strictly positive. Pick $\mathcal{L} = L\sqrt{\mathcal{D}}$, which is lower triangular.

□

2 Exercise 1.

Compute the Cholesky factorization for the below matrix:

$$\begin{bmatrix} 4 & 12 & -16 \\ 12 & 37 & -43 \\ -16 & -43 & 98 \end{bmatrix} \tag{14}$$

3 Exercise 2.

Consider a recurrent system of equations:

$$T_i = 1 + pT_{i+1} + qT_{i-1} \tag{15}$$

for $i = 1, 2 \cdots N$ with two boundary values $T_0 = 0$ and $T_N = 0$. Construct a linear system equivalent to the above recurrent equations in the form of $AT = b$, and use LU factorization to solve for T.

References

[1] G. H. Golub and C. F. Van Loan, *Matrix computations*. JHU press, 2013.

[2] L. N. Trefethen and D. Bau III, *Numerical linear algebra*. Siam, 1997, vol. 50.