Symmetric positive-definite matrices I

**Definition**

A symmetric matrix $A \in \mathbb{R}^{n \times n}$ is positive definite iff $x^T A x > 0$ holds $\forall x \neq 0 \in \mathbb{R}^n$.

Such matrices naturally arise in a variety of math, science, and engineering applications. For example,

- The Hamiltonian operator of a physical system
- The Hessian of a convex function
- The covariance matrix of linearly independent random variables
Theorem

The following statements are equivalent:

1. $A$ is symmetric positive definite.
2. $(x, y) := x^T A y$ is an inner product on $\mathbb{R}^n$.
3. All eigenvalues are positive and eigenvectors can be constructed to form an orthonormal basis.
4. $A$ is symmetric with positive leading principal minors.
5. The Cholesky decomposition of $A$ exists.
Existence I

To prove the existence of the Cholesky decomposition for symmetric positive definite matrices, we apply induction.

- Induction hypothesis: Given any spd $A_{n-1} \in \mathbb{R}^{n-1 \times n-1}$ assume there exists lower-triangular $L_{n-1}$ where

$$A_{n-1} = L_{n-1}L_{n-1}^T$$

- Base case: $A_1 = [a_{1,1}] = [\sqrt{a_{1,1}}][\sqrt{a_{1,1}}]^T$.

- Consistency: Show that for any spd $A_n \in \mathbb{R}^{n \times n}$ there exists $L_n$ such that

$$A_n = L_nL_n^T$$
Existence II

Let us represent $A_n$ as

$$A_n = \begin{bmatrix} \alpha & c^T \\ c & B \end{bmatrix}$$

where $\alpha := a_{1,1}$ is a scalar, $c := a_{2:n,1}$ is a column vector, and $B = a_{2:n,2:n}$ is the remaining $\mathbb{R}^{n-1 \times n-1}$ lower-right sub-matrix. Then we have

$$A_n = \begin{bmatrix} \frac{\sqrt{\alpha}}{\sqrt{\alpha}c} & 0 \\ 0 & I_{n-1} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ B - \frac{1}{\alpha}cc^T \end{bmatrix} \begin{bmatrix} \frac{\sqrt{\alpha}}{\sqrt{\alpha}c^T} \\ 0 & I_{n-1} \end{bmatrix}$$
Existence III

Let $y$ be an arbitrary nonzero column vector in $\mathbb{R}^{n-1}$. We can solve

$$\begin{bmatrix} \sqrt{\alpha} & \frac{1}{\sqrt{\alpha}} c^T \\ 0 & I_{n-1} \end{bmatrix} x = \begin{bmatrix} 0 \\ y \end{bmatrix}$$

It follows

$$y^T (B - \frac{1}{\sqrt{\alpha}} cc^T)y = x^T A_n x > 0$$

Thus $B - \frac{1}{\alpha} cc^T$ is spd. From the induction hypothesis

$$B - \frac{1}{\alpha} cc^T = L_{n-1} L_{n-1}^T$$
Putting it all together, we have

\[
A_n = \begin{bmatrix}
\sqrt{\alpha} & 0 \\
\frac{1}{\sqrt{\alpha}}c & I_{n-1}
\end{bmatrix}
\begin{bmatrix}
1 & 0 \\
0 & B - \frac{1}{\alpha}cc^T
\end{bmatrix}
\begin{bmatrix}
\sqrt{\alpha} & \frac{1}{\sqrt{\alpha}}c^T \\
0 & I_{n-1}
\end{bmatrix}
\]

\[
= \begin{bmatrix}
\sqrt{\alpha} & 0 \\
\frac{1}{\sqrt{\alpha}}c & I_{n-1}
\end{bmatrix}
\begin{bmatrix}
1 & 0 \\
0 & L_{n-1}L_{n-1}^T
\end{bmatrix}
\begin{bmatrix}
\sqrt{\alpha} & \frac{1}{\sqrt{\alpha}}c^T \\
0 & I_{n-1}
\end{bmatrix}
\]

\[
= \begin{bmatrix}
\sqrt{\alpha} & 0 \\
\frac{1}{\sqrt{\alpha}}c & L_{n-1}
\end{bmatrix}
\begin{bmatrix}
\sqrt{\alpha} & \frac{1}{\sqrt{\alpha}}c^T \\
0 & L_{n-1}^T
\end{bmatrix}
\]

\[
= L_nL_n^T
\]
Note that the proof of existence was constructive. That means we can follow the same procedure to calculate the Cholesky decomposition.

1. Loop over columns.
   \[ \text{for } k=1:n-1 \]

2. Set diagonal element of \( L \).
   \[ L(k,k) = \sqrt{A(k,k)} \]

3. Finish column.
   \[ L(k+1:n,k) = A(k+1:n) / L(k,k) \]

4. Update lower right sub-matrix of \( A \).
   \[ A(k+1:n,k+1:n) = A(k+1:n,k+1:n) - L(k+1:n,k)^T \]

5. End for loop.
   \[ \text{end} \]
We can similarly take advantage of the structure of band matrices to optimize the calculation of the LU decomposition.

**Definition**

A band matrix $A \in \mathbb{R}^{n \times n}$ of band width $2m + 1$ has nonzero entries only on the main diagonal, $m$ super-diagonals, and $m$ sub-diagonals.
Band matrices II

For example, a tridiagonal matrix (band width 3) has the form:

\[ A = \begin{bmatrix}
    a_{1,1} & a_{1,2} & & & \\
    a_{2,1} & a_{2,2} & a_{2,3} & & \\
    & a_{3,2} & a_{3,3} & a_{3,4} & \\
    & & a_{4,3} & a_{4,4} & \cdots \\
    & & & \cdots & \cdots \\
    0 & & & & a_{n-1,n} \\
    & & & & a_{n,n-1}
\end{bmatrix} \]
We can easily show that the LU decomposition will have the form:

\[
A = \begin{bmatrix}
1 & & & 0 \\
(l_{2,1}) & 1 & & \\
& \ddots & \ddots & \\
0 & \cdots & (l_{n,n-1}) & 1 \\
\end{bmatrix} \begin{bmatrix}
u_{1,1} & u_{1,2} & & 0 \\
um_{1,1} & u_{2,2} & \cdots & \\
& \ddots & \ddots & \\
0 & \cdots & u_{n-1,n} & u_{n,n} \\
\end{bmatrix}
\]

Because we know so many entries must be zero, we can optimize the algorithm to avoid calculating them. Similarly, the procedures for forward and backward substitution can also be optimized in these cases.
Partial pivoting can be implemented, but it will increase the band width of $U$ from $m + 1$ to $2m + 1$. However, pivoting can sometimes be avoided.

**Definition**

A matrix $A \in \mathbb{R}^{n\times n}$ is column diagonally dominant iff

$$|a_{j,j}| > \sum_{i \neq j} |a_{i,j}|$$

We can show that a column diagonally dominant matrix never requires pivoting.
Diagonal dominance II

Proof: Let $a_{k,j}^{(i)}$ represent element $k, j$ after zeroing column $i$ in the standard LU algorithm. Assume the induction hypothesis:

$$|a_{j,j}^{(i)}| > \sum_{k=i+1, k \neq j}^{n} |a_{k,j}^{(i)}|$$

When column $i + 1$ is zeroed below the diagonal, the elements of $A$ update as follows:

$$a_{k,j}^{(i+1)} = a_{k,j}^{(i)} - \frac{a_{k,i}^{(i)} a_{i+1,j}^{(i)}}{a_{i+1,i}^{(i)}}$$
Diagonal dominance III

\[ |a_{j,j}^{(i+1)}| = |a_{j,j}^{(i)}| - \frac{a_{j,i+1}^{(i)}a_{i+1,j}^{(i)}}{a_{i+1,i+1}} \]

\[ \geq |a_{j,j}^{(i)}| - \frac{|a_{j,i+1}^{(i)}||a_{i+1,j}^{(i)}|}{|a_{i+1,i+1}|} \]

\[ > \sum_{k=i+1, k \neq j}^{n} |a_{k,j}^{(i)}| - \frac{|a_{j,i+1}^{(i)}||a_{i+1,j}^{(i)}|}{|a_{i+1,i+1}|} \]

\[ = \sum_{k=i+2, k \neq j}^{n} |a_{k,j}^{(i)}| + |a_{i+1,j}^{(i)}| \left(1 - \frac{|a_{j,i+1}^{(i)}|}{|a_{i+1,i+1}|}\right) \]
Diagonal dominance IV

To make further progress we observe:

\[
|a_{k,j}^{(i+1)}| \leq |a_{k,j}^{(i)}| + \frac{|a_{k,i+1}^{(i)}||a_{i+1,j}^{(i)}|}{|a_{i+1,i+1}^{(i)}|}
\]

\[
|a_{k,j}^{(i)}| \geq |a_{k,j}^{(i+1)}| - \frac{|a_{k,i+1}^{(i)}||a_{i+1,j}^{(i)}|}{|a_{i+1,i+1}^{(i)}|}
\]
Together this gives:

\[
|a_{j,j}^{(i+1)}| > \sum_{k=i+2, \neq j}^{n} |a_{k,j}^{(i+1)}| + |a_{i+1,j}^{(i)}| \left(1 - \sum_{k=i+2}^{n} \frac{|a_{k,i+1}^{(i)}|}{|a_{i+1,i+1}^{(i)}|}\right)
\]

> \sum_{k=i+2, \neq j}^{n} |a_{k,j}^{(i+1)}|}

This shows consistency for the induction hypothesis and the base case easily follows from the definition of diagonal dominance. The desired result immediate follows since the diagonal elements are always largest in magnitude.
We can follow the standard LU procedure and simply avoid elements that do not update. If $A$ has band width $2m + 1$, we have

1. Loop over columns.
   
   \[ \text{for } k=1:n-1 \]

2. Construct column $k$ of $L$.
   
   \[ L(k+1:k+m,k) = A(k+1:k+m,k)/A(k,k) \]

3. Set column $k$ of $A$ to zero.
   
   \[ A(k+1:k+m,k) = 0 \]

4. Update lower right sub-matrix of $A$.
   
   \[ A(k+1:k+m,k+1:k+m) = A(k+1:k+m,k+1:k+m) - L(k+1:k+m,k)*A(k,k+1:k+m) \]

5. End for loop. Identify $U$.
   
   end; $U = A$
In the case of a tridiagonal matrix, the procedure becomes exceptionally simple and efficient. Let us write the diagonals of $A$ as vectors. Then $L$ and $U$ can be written as:

$$A = \begin{bmatrix}
  d_1 & e_1 & 0 \\
  c_1 & d_2 & \ddots \\
  0 & c_{n-1} & d_n
\end{bmatrix}$$

$$= \begin{bmatrix}
  1 & 0 \\
  l_1 & 1 \\
  0 & l_{n-1} & 1
\end{bmatrix} \begin{bmatrix}
  u_1 & e_1 & 0 \\
  u_2 & \ddots \\
  0 & \ddots & e_{n-1} \\
  & & u_n
\end{bmatrix}$$
Follow the same procedure, but avoid updating $A$. Build $U$ directly. Note that the super-diagonal doesn’t change and can be copied directly into $U$.

1. Set first row of $U$
   \[ u(1) = d(1) \]

2. Loop over columns.
   \[ \text{for } k = 1:n-1 \]

3. Construct column $k$ of $L$.
   \[ l(k) = c(k)/u(k) \]

4. Update $A$ and place result directly in $U$.
   \[ u(k+1) = d(k+1) - l(k) \times e(k) \]

5. End for loop.
   \[ \text{end} \]