Cholesky factorization

Positive definite matrices

Cholesky decomposition

Let a real matrix $\mathbf{A}$ is

symmetric: $\mathbf{A}^T = \mathbf{A}$

positive definite: $\mathbf{x}^T \mathbf{A} \mathbf{x} > 0 \quad \forall \mathbf{x} \in \mathbb{R}^m$

Then

$$\mathbf{A} = \mathbf{L}\mathbf{L}^T$$

where $\mathbf{L}$ is a lower triangular matrix.

Cholesky decomposition

$$
\begin{aligned}
\mathbf{A} &= \mathbf{L}\mathbf{L}^T \\
&= \begin{pmatrix} l_{11} & 0 & 0 & \cdots & 0 \\ l_{21} & l_{22} & 0 & \cdots & 0 \\ l_{31} & l_{32} & l_{33} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \\ l_{m1} & l_{m2} & l_{m3} & \cdots & l_{mm} \end{pmatrix} \begin{pmatrix} l_{11} & l_{21} & l_{31} & \cdots & l_{m1} \\ 0 & l_{22} & l_{32} & \cdots & l_{m2} \\ 0 & 0 & l_{33} & \cdots & l_{m3} \\ \vdots & \vdots & & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & l_{mm} \end{pmatrix}
\end{aligned}
$$

1st row of $\mathbf{A}$

$$
\begin{aligned}
a_{11} &= l_{11}^2 \\
a_{12} &= l_{11}l_{21}, \quad \cdots, \quad a_{1k} = l_{11}l_{k1}, \quad k = 2, \ldots, m
\end{aligned}
$$

NB: The square root is OK because $\mathbf{A}$ is positive definite.

Cholesky decomposition

$$\mathbf{A} = \mathbf{L}\mathbf{L}^T$$

$$= \begin{pmatrix} l_{11} & 0 & 0 & \cdots & 0 \\ l_{21} & l_{22} & 0 & \cdots & 0 \\ l_{31} & l_{32} & l_{33} & \cdots & 0 \\ \vdots & \vdots & \vdots & \ddots & \\ l_{m1} & l_{m2} & l_{m3} & \cdots & l_{mm} \end{pmatrix} \begin{pmatrix} l_{11} & l_{21} & l_{31} & \cdots & l_{m1} \\ 0 & l_{22} & l_{32} & \cdots & l_{m2} \\ 0 & 0 & l_{33} & \cdots & l_{m3} \\ \vdots & \vdots & & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & l_{mm} \end{pmatrix}$$

2nd row of $\mathbf{A}$

$$a_{21} = l_{21}l_{11}$$

$$a_{22} = l_{21}^2 + l_{22}^2, \quad \cdots, \quad a_{2k} = l_{21}l_{k1} + l_{22}l_{k2}, \quad k = 2, \ldots, m$$

NB: The square root is OK because $\mathbf{A}$ is positive definite.

Cholesky decomposition

Compared to a general $\mathbf{LU}$ factorization, Cholesky decomposition:

- requires $1/2$ memory
- requires $\sim 1/2$ less operations
- has better stability, and does *not* require pivoting
- fails if $\mathbf{A}$ is not PD.

Systems of linear equations

If $\mathbf{A}$ is symmetric and positive definite, then

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

is solved via $\mathbf{A} = \mathbf{L}\mathbf{L}^T$, and

$$\begin{aligned} \mathbf{L}\mathbf{y} &= \mathbf{b} \qquad \text{(forward substitution)} \\ \mathbf{L}^T\mathbf{x} &= \mathbf{y} \qquad \text{(back substitution)} \end{aligned}$$

Applications of Cholesky decomposition

Quantum mechanics

Observables are represented by Hermitian operators. ($\left(\mathbf{A}^T\right)^* = \mathbf{A}$)

Applications of Cholesky decomposition

Numerical optimization

The Hessian matrix of a multivariate function $F(\mathbf{x})$

$$H_{jk} = \frac{\partial^2 F}{\partial x_j \partial x_k}$$

is symmetric and is in some cases positive (semi-)definite.

Applications of Cholesky decomposition

Monte Carlo simulations

Generation of correlated Gaussian random variables: decompose the correlation matrix $\mathbf{C} = \mathbf{L}\mathbf{L}^T$, generate a vector of uncorrelated values $\mathbf{x}$, then

$$\mathbf{z} = \mathbf{L}\mathbf{x}$$

has the correlation matrix $\mathbf{C}$.