Part 2c: Simulating multivariate normal vectors

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Simulating from the multivariate normal

(a) Find a matrix A such that $\Sigma = AA^T$, for example using the Cholesky decomposition of A.

(b) Generate independent random values $X_1, X_2, \ldots, X_d \sim \mathcal{N}(0, 1)$.

(c) Return $AX + \mu$.

The Cholesky decomposition (Wikipedia)

The Cholesky decomposition of a Hermitian positive-definite matrix **A**, is a decomposition of the form

$$\mathbf{A} = \mathbf{L}\mathbf{L}^*,$$

where **L** is a lower triangular matrix with real and positive diagonal entries, and **L*** denotes the conjugate transpose of **L**. Every Hermitian positive-definite matrix (and thus also every real-valued symmetric positive-definite matrix) has a unique Cholesky decomposition.[3]

The converse holds trivially: if **A** can be written as **LL*** for some invertible **L**, lower triangular or otherwise, then **A** is Hermitian and positive definite.

When **A** is a real matrix (hence symmetric positive-definite), the factorization may be written

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

where **L** is a real lower triangular matrix with positive diagonal entries.[4][5][6]

The Cholesky decomposition (an example)

$$\Sigma = \begin{pmatrix} 6 & 15 & 55 \\ 15 & 55 & 225 \\ 55 & 225 & 979 \end{pmatrix} = \left(\sigma_{ij}\right)$$

$$L_{11} = \sqrt{\sigma_{11}} = \sqrt{6} \simeq 2.4495, \quad L_{12} = L_{13} = 0$$

$$L_{21} = \frac{\sigma_{21}}{L_{11}} \simeq \frac{15}{2.4495} \simeq 6.1237$$

$$L_{22} \simeq \sqrt{\sigma_{22} - L_{21}^2} \simeq \sqrt{55 - (6.1237)^2} = 4.1833, \quad L_{23} = 0$$

$$L_{31} = \frac{\sigma_{31}}{L_{11}} = \frac{55}{2.4495} \simeq 22.4537$$

$$L_{32} = \sqrt{\sigma_{32} - L_{31} \times L_{21}} = 20.9165$$

$$L_{33} \simeq \sqrt{\sigma_{33} - L_{31}^2 - L_{32}^2} \simeq 6.1101$$

$$L = \begin{pmatrix} 2.4495 & 0 & 0 \\ 6.1237 & 4.1833 & 0 \\ 22.4537 & 20.9165 & 6.1101 \end{pmatrix}, \quad LL^T = \Sigma$$

$$\vec{Y} = L\vec{X} + \vec{\mu} \Rightarrow \vec{Y} \sim N(\vec{\mu}, \Sigma)$$

The spectral decomposition

Every real symmetric $n \times n$ matrix can be factored as

$$\Sigma = U \Lambda U^T$$

- U = orthogonal matrix of eigenvectors.
- Λ = diagonal matrix of eigenvalues.

$$p(\lambda) = \det(\Sigma - \lambda I) \Rightarrow p(\lambda_i) = 0, \quad 1 \leq i \leq d$$

$$U = (\vec{u}_1, \vec{u}_2, \ldots, \vec{u}_d), \qquad \Sigma \vec{u}_i = \lambda_i \vec{u}_i$$

also, $\vec{u}_i^T \vec{u}_j = 0, \quad i \neq j, \quad \|\vec{u}_i\|^2 = 1$

$$\Lambda = \begin{pmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_d \end{pmatrix}$$

$$\Sigma^{1/2} = U \Lambda^{1/2} U^T, \quad \Lambda^{1/2} = \begin{pmatrix} \sqrt{\lambda_1} & & & 0 \\ & \sqrt{\lambda_2} & & \\ & & \ddots & \\ 0 & & & \sqrt{\lambda_d} \end{pmatrix}$$

$$\Sigma^{1/2} (\Sigma^{1/2})^T = (\Sigma^{1/2})^2 = \Sigma$$

$$\vec{y} = \Sigma^{1/2} \vec{x} + \vec{\mu} \Rightarrow \vec{y} \sim N(\vec{\mu}, \Sigma)$$

The spectral decomposition (an example)

$$\Sigma = \begin{pmatrix} 6 & 15 & 55 \\ 15 & 55 & 225 \\ 55 & 225 & 970 \end{pmatrix}$$

$$\Lambda = \begin{pmatrix} 1034.03 & 0 & 0 \\ 0 & 5.244 & 0 \\ 0 & 0 & 0.721 \end{pmatrix}$$

$$U = \begin{pmatrix} -0.055 & -0.684 & 0.728 \\ -0.224 & -0.702 & -0.676 \\ -0.973 & 0.201 & 0.115 \end{pmatrix}$$

$$\Lambda^{1/2} = \begin{pmatrix} 32.156 & 0 & 0 \\ 0 & 2.290 & 0 \\ 0 & 0 & 0.850 \end{pmatrix}$$

$$\Sigma^{1/2} = U \Lambda^{1/2} U^{T} = \begin{pmatrix} 1.619 & 1.079 & 1.488 \\ 1.079 & 3.136 & 6.633 \\ 1.488 & 6.633 & 30.542 \end{pmatrix}$$