POSITIVE DEFINITENESS AND POSITIVE SEMIDEFINITENESS

Positive definiteness is a linear algebra concept that arises in different fields; a positive definite matrix can be considered analogous to a positive number. The definition of a positive definite matrix is a symmetric matrix $A$ such that

$$x^T Ax > 0$$

for all nonzero vectors $x \in \mathbb{R}^n$, where $x^T$ is the transpose of vector $x$.

Some common applications of positive definite matrices appear in optimization algorithms, the construction of linear regression models, and testing for the strict convexity of scalar-valued vector functions (using the positive definiteness of the Hessian). Characterizations of positive definite matrices include positive eigenvalues and positive leading principal minors.

A positive semi-definite matrix is defined as a symmetric matrix $B$ such that

$$x^T Bx \geq 0$$

for all vectors $x \in \mathbb{R}^n$.

Positive semi-definiteness can be considered a generalization of positive definiteness since it allows $x^T Bx$ to equal 0. It also allows $B$ to be a singular matrix, in which case $B$ will have at least one zero eigenvalue.
COVARIANCE MATRICES

In statistics, a covariance matrix is a generalization of the measure of variance to higher dimensions. A covariance matrix is a matrix of covariances between elements of a random vector $X$. If we define $X$ as an $n \times 1$ vector with random variables $x_i$ as entries, then the covariance matrix $\Sigma$ is a matrix with covariances $\sigma_{ij} = \text{E}[(x_i - \mu_i)(x_j - \mu_j)]$ as entries, where $\mu_i = \text{E}(x_i)$ and can be written using matrix notation as:

$$
\Sigma = \text{E}[(X - \mu)(X - \mu)^T] = \begin{bmatrix}
\sigma_{11} & \sigma_{12} & \cdots & \sigma_{1n} \\
\sigma_{21} & \sigma_{22} & \cdots & \sigma_{2n} \\
\vdots & \vdots & \ddots & \vdots \\
\sigma_{n1} & \sigma_{n2} & \cdots & \sigma_{nn}
\end{bmatrix}.
$$

In the above notation, $\Sigma$ is equal to $\text{cov}(X, X)$, which is equal to $\text{var}(X)$. This comes from the definition of variance for a univariate random variable $w$, such as $\text{var}(w) = \text{E}[(w - \mu)^2]$.

Covariances are symmetric, so $\text{cov}(X, X_i) = \text{cov}(X_i, X)$; therefore, covariance matrices are symmetric. If $Y$ is a vector of random variables such that $Y = \alpha^T X$ for an $n \times 1$ vector of constants $\alpha$, then the covariance matrix for $Y$ is equal to

$$
\text{var}(Y) = \text{cov}(Y, Y) = \text{cov}(\alpha^T X, \alpha^T X) = \text{cov}\left(\sum_{i=1}^{n} \alpha_i x_i, \sum_{j=1}^{n} \alpha_j x_j\right) = \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j \text{cov}(x_i, x_j)
$$

$$
= \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j \sigma_{ij} = \alpha^T \Sigma \alpha \geq 0.
$$

Since this is true for any choice of $\alpha$, this shows that any given covariance matrix is at least positive semi-definite (Schott, 1997).