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Consider two covariance matrices $\mathbf{A}_{n\times n}$ and $\mathbf{B}_{n\times n}$. We say that \mathbf{A} is *bigger* than \mathbf{B} , often denoted by $\mathbf{A} \geq \mathbf{B}$ or $\mathbf{A} \succeq \mathbf{B}$, if $\mathbf{A} - \mathbf{B}$ is semi-positive definite. Why do we use the "definiteness" of a matrix to compare the size of two covariance matrices?

First, notice that a covariance matrix is not only symmetrical, but also semi-positive definite. Consider a random vector $\mathbf{x} = (x_1, ..., x_n)^{\top}$. The covariance matrix is defined by

$$\mathbf{K} \coloneqq \mathbf{E}[(\mathbf{x} - \mathbf{E}[\mathbf{x}])(\mathbf{x} - \mathbf{E}[\mathbf{x}])^{\top}].$$

Given any constant vector \mathbf{v} of length n, we have

$$\mathbf{v}^{\top} \mathbf{K} \mathbf{v} = \mathbf{E}[\mathbf{v}^{\top} (\mathbf{x} - \mathbf{E}[\mathbf{x}]) (\mathbf{v}^{\top} (\mathbf{x} - \mathbf{E}[\mathbf{x}]))^{\top}] \ge 0$$

by the definition of K. Therefore, the covariance matrix K is semi-positive definite. In fact, $\mathbf{v}^{\top} K \mathbf{v}$ is zero iff \mathbf{x} has no variance at all.

There is another intuitive way of interpreting the definiteness described above. Consider the same vector \mathbf{v} and the random vector \mathbf{x} . The dot product $\mathbf{v}^{\top}\mathbf{x}$ is the projection of the random vector from n-dimensional space on a one-dimensional space along the direction of \mathbf{v} , i.e., this collapse the n-dimensional random variable to a one-dimensional random variable through some linear combination. If we calculate the variance of the one-dimensional random variable $\mathbf{v}^{\top}\mathbf{x}$, we obtain

$$\begin{aligned} \operatorname{Var}[\mathbf{v}^{\top}\mathbf{x}] &= \mathbf{E}[\mathbf{v}^{\top}\mathbf{x}(\mathbf{v}^{\top}\mathbf{x})^{\top}] - \mathbf{E}[\mathbf{v}^{\top}\mathbf{x}] \, \mathbf{E}[\mathbf{v}^{\top}\mathbf{x}]^{\top} \\ &= \mathbf{v}^{\top} \big(\, \mathbf{E}[\mathbf{x}\mathbf{x}^{\top}] - \mathbf{E}[\mathbf{x}] \, \mathbf{E}[\mathbf{x}]^{\top} \big) \mathbf{v} \\ &= \mathbf{v}^{\top} \mathbf{K} \mathbf{v}. \end{aligned}$$

Notice that the variance assumes the exact form as before. And since variance is non-negative, it is clear that the covariance matrix must be semi-positive definite. That is, for any direction \mathbf{v} , the variance of " \mathbf{x} projected on that direction" is (clearly) non-negative.

Motivated by the intuitive interpretation, lets now compare two covariance matrices. Let $\mathbf{x} = (x_1,...,x_n)^{\top}$ and $\mathbf{y} = (y_1,...,y_n)^{\top}$ be random vectors with mean $(0,...,0)^{\top}$ for simplicity. Let $\mathbf{A} = \mathbf{E}[\mathbf{x}\mathbf{x}^{\top}]$ and $\mathbf{B} = \mathbf{E}[\mathbf{y}\mathbf{y}^{\top}]$ be the covariance matrices. Our goal is to compare \mathbf{A} and \mathbf{B} in some meaningful way. We can project \mathbf{x} and \mathbf{y} on a vector \mathbf{v} , and then compare the variance (non-negative real number) of the two projections. To make the comparison

meaningful, it is reasonable to compare all possible projections, i.e., consider all possible choices of \mathbf{v} .

Formally, consider any vector \mathbf{v} . The projection of \mathbf{x} on \mathbf{v} is $\mathbf{v}^{\top}\mathbf{x}$. The variance of $\mathbf{v}^{\top}\mathbf{x}$ is

$$\begin{split} \mathbf{E}[(\mathbf{v}^{\top}\mathbf{x})^2] &= \mathbf{E}[\mathbf{v}^{\top}\mathbf{x}\mathbf{x}^{\top}\mathbf{v}] \\ &= \mathbf{v}^{\top}\,\mathbf{E}[\mathbf{x}\mathbf{x}^{\top}]\mathbf{v} = \mathbf{v}^{\top}\mathbf{A}\mathbf{v} \end{split}$$

where **A** is the covariance matrix. Similarly, consider the same for **y**. If we find that \forall **v**,

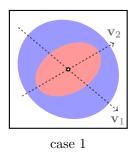
$$\mathbf{v}^{\top} \mathbf{A} \mathbf{v} - \mathbf{v}^{\top} \mathbf{B} \mathbf{v} = \mathbf{v}^{\top} (\mathbf{A} - \mathbf{B}) \mathbf{v} \ge 0,$$

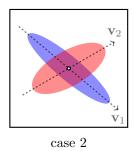
then, by definition, $\mathbf{A} - \mathbf{B}$ is semi-positive definite. Now we know why we say \mathbf{A} is *larger* than \mathbf{B} when $\mathbf{A} - \mathbf{B}$ is positive definite:

If $\mathbf{A} - \mathbf{B}$ is positive definite, then for all possible directions \mathbf{v} , the variance of \mathbf{x} is larger than \mathbf{y} 's.

 $^a{\rm This}$ order of semi-positive definite matrices is called the Löwner ordering.

This interpretation of the partial ordering can be understood easily through visualisation. The following are representations of the distributions ${\bf x}$ and ${\bf y}$ where the two random vectors are two-dimensional:





Let \mathbf{x} with covariance matrix \mathbf{A} be the blue distribution and \mathbf{y} with covariance matrix \mathbf{B} be the red distribution. It is clear that in case 1, \mathbf{A} is bigger than \mathbf{B} since the variance of \mathbf{x} is bigger that \mathbf{y} 's in every direction. (every possible direction of projection) However, the same statement is not true in case 2. In some directions (e.g. \mathbf{v}_1), the variance of \mathbf{x} is larger; in other directions (e.g. \mathbf{v}_2), the variance of \mathbf{y} is larger. Thus, \mathbf{A} and \mathbf{B} are not comparable by the partial order in case 2.