Overlap matrix

1. Let $\{\mathbf{x}_i\}$ ($i = 1,...N$) be a set of vectors belonging to any vector space of any dimension with scalar product $(\cdot,\cdot)$. We can construct a matrix **S** (referred to as *overlap matrix*) with the following matrix elements:

$$S_{ij} = (\mathbf{x}_i, \mathbf{x}_j)$$

2. From the properties of the scalar product it follows that the overlap matrix is *Hermitian*:

$$S_{ji} = (\mathbf{x}_j, \mathbf{x}_i) = \overline{(\mathbf{x}_i, \mathbf{x}_j)} = \overline{S_{ij}} \Rightarrow \mathbf{S} = \mathbf{S}^\dagger$$

3. The overlap matrix is *non-singular* if and only if the vector set $\{\mathbf{x}_i\}$ is linearly independent. The proof should be done in two parts:

(**a**) Let us prove that if $\{\mathbf{x}_i\}$ is linearly dependent, the matrix **S** is singular.
The linear dependence means that there exists a set of coefficients $\alpha_1, \alpha_2,... \alpha_N$ such that at least one of them is not zero and:

$$\sum_{i=1}^{N} \alpha_i \mathbf{x}_i = \mathbf{0}$$

Multiplying (in the sense of scalar product) by $\mathbf{x}_k$ we obtain:

$$\sum_{i=1}^{N} \alpha_i (\mathbf{x}_k, \mathbf{x}_i) = \mathbf{0} \Rightarrow \sum_{i=1}^{N} S_{ki}\alpha_i = \mathbf{0}$$

Since this is true for any k, this means (in matrix-vector notations) that $\mathbf{S}\alpha = \mathbf{0}$. This, there exists a non-zero vector α that is turned by matrix **S** to zero. Thus, **S** is singular by definition.

(**b**) Now we prove that if **S** is singular, then $\{\mathbf{x}_i\}$ is linearly dependent. This is done essentially by inverting the previous proof. Since **S** is singular, there exists a non-zero vector α that is turned by matrix **S** to zero: $\mathbf{S}\alpha = \mathbf{0}$. Thus,

$$\sum_{i=1}^{N} S_{ki}\alpha_i = \mathbf{0} \Rightarrow \sum_{i=1}^{N} (\mathbf{x}_k, \mathbf{x}_i)\alpha_i = \mathbf{0} \Rightarrow \sum_{i=1}^{N} \alpha_i (\mathbf{x}_k, \mathbf{x}_i) = 0 \Rightarrow (\mathbf{x}_k, \sum_{i=1}^{N} \alpha_i \mathbf{x}_i) = 0$$ This is true for any k. Multiplying the latter expression by α_k and summing over all k, we obtain:

$$\sum_{k=1}^{N} \alpha_k (\mathbf{x}_k, \sum_{i=1}^{N} \alpha_i \mathbf{x}_i) = \sum_{k=1}^{N} (\alpha_k \mathbf{x}_k, \sum_{i=1}^{N} \alpha_i \mathbf{x}_i) = (\sum_{k=1}^{N} \alpha_k \mathbf{x}_k, \sum_{i=1}^{N} \alpha_i \mathbf{x}_i) = 0$$

Note that the latter expression is a scalar square:

$$(\sum_{k} \alpha_k \mathbf{x}_k, \sum_{i} \alpha_i \mathbf{x}_i) = (\sum_{i} \alpha_i \mathbf{x}_i, \sum_{i} \alpha_i \mathbf{x}_i) = (\mathbf{v}, \mathbf{v})$$

where the vector $\mathbf{v} = \sum_i \alpha_i \mathbf{x}_i$. Since $(\mathbf{v},\mathbf{v}) = 0$ if and only if $\mathbf{v} = 0$, it follows that $\sum_i \alpha_i \mathbf{x}_i = \mathbf{0}$. Since not all α_i's are zeros, this means that $\{\mathbf{x}_i\}$ is a linearly dependent set. **QED**

4. If the vector set $\{\mathbf{x}_i\}$ is linearly independent, the overlap matrix **S** is *positive definite*. We will essentially prove that the corresponding quadratic form $(\mathbf{Sy},\mathbf{y})$ is positive definite, i.e., that it is positive for any non-zero vector **y**: $\forall \mathbf{y} \neq 0 \ \ (\mathbf{Sy}, \mathbf{y}) > 0$:

$$(\mathbf{Sy}, \mathbf{y}) = \sum_{i}\sum_{j} S_{ij} \overline{y_i} y_j = \sum_{i}\sum_{j} (\mathbf{x}_i, \mathbf{x}_j) \overline{y_i} y_j = \sum_{i}\sum_{j} (\overline{y_i}\mathbf{x}_i, \overline{y_j}\mathbf{x}_j)$$

$$= (\sum_{i} \overline{y_i}\mathbf{x}_i, \sum_{j} \overline{y_j}\mathbf{x}_j)$$

The latter expression is a scalar square which is can be only *positive* or *zero*. If it is positive $\Rightarrow$ **QED**. If it is zero, it means that $\sum_i \overline{y_i}\mathbf{x}_i = 0$. Since $\mathbf{y} \neq 0$, it follows that $\{\mathbf{x}_i\}$ is linearly dependent, which is not true. Thus, the only possibility for a linearly independent set $\{\mathbf{x}_i\}$ is that $(\mathbf{Sy},\mathbf{y})>0$ for any non-zero vector $\mathbf{y}$. Thus, **S** is positive definite and all its eigenvalues will be positive (note that they are all real due to hermiticity of **S**). **QED**

5. If we drop the linear independence condition from the previous statement, we will see that $\forall\mathbf{y}\ \ (\mathbf{Sy},\mathbf{y}) \geq 0$. Thus, in this case **S** is *positive-semidefinite* (sometimes called *nonnegative-definite*). In terms of the eigenvalues, it means that all the eigenvalues are non-negative (positive or zero). The proof is essentially given in the previous section.