Let $T \in \text{Hom}(V, V)$, where V is a finite-dimensional inner product space over $\mathbb{F}$. Define T as positive semi-definite if $T = T^*$ and $\langle T(x), x\rangle \geq 0$ for all $x \in V$.

Lemma 0.1

If $T = T^*$, then T is positive semi-definite if and only if all eigenvalues of T are in $\mathbb{R}^+ \cup \{0\}$.

Proof.

Assume $T = T^*$.

Suppose first T is positive semi-definite, i.e. $\langle T(x), x\rangle \geq 0$ for all $x \in V$.

Let λ be an arbitrary eigenvalue of T. Thus, for a corresponding eigenvector $x \in V$, $Tx = \lambda x$.

Since T is self-adjoint, then all the eigenvalues are real.

Since T is positive semi-definite, then $\langle \lambda x, x\rangle = \lambda\langle x, x\rangle \geq 0$.

Thus, since x is an eigenvector, $x \neq 0$, then $\langle x, x\rangle > 0$ and hence $\lambda \geq 0$. Suppose now any eigenvalue λ is such that $\lambda \in \mathbb{R}^+ \cup \{0\}$.

Since T is self-adjoint and $\mathbb{F} = \mathbb{C}$ or $\mathbb{F} = \mathbb{R}$, then by the Spectral Theorem there is an orthonormal basis β of V, consisting of eigenvectors of T. Let v be an arbitrary vector of β.

Note that $Tv = \lambda v$ for some $\lambda \in \mathbb{R}^+ \cup \{0\}$ by assumption.

Take an arbitrary $x \in V$. Since β is a basis, there exist $a_1, a_2, \ldots, a_n \in \mathbb{F}$, where $n = \dim V$, such that, for $v_i \in \beta$ and λ_i being a corresponding eigenvalue,

$$v = \sum_{i=1}^{n} a_i v_i.$$

Consider $\langle Tx, x\rangle$:

$$\begin{aligned}
\langle Tx, x\rangle &= \langle T(\sum_{i=1}^{n} a_i v_i), \sum_{j=1}^{n} a_j v_j\rangle && (1)\\
&= \langle \sum_{i=1}^{n} a_i T(v_i), \sum_{j=1}^{n} a_j v_j\rangle && (2)\\
&= \langle \sum_{i=1}^{n} a_i \lambda_i v_i, \sum_{j=1}^{n} a_j v_j\rangle && (3)\\
&= \sum_{i=1}^{n} a_i \lambda_i \langle v_i, \sum_{j=1}^{n} a_j v_j\rangle && (4)\\
&= \sum_{i=1}^{n} a_i \lambda_i \sum_{j=1}^{n} \overline{a_j} \langle v_i, v_j\rangle && (5)\\
&= \sum_{i=1}^{n} a_i \lambda_i \sum_{j=1}^{n} \overline{a_j} \langle v_i, v_j\rangle && (6)\\
&= \sum_{i=1}^{n} a_i \lambda_i \sum_{j=1}^{n} \overline{a_j} \delta_{ij} && (7)
\end{aligned}$$

$$= \sum_{i=1}^{n} \left| a_i^2 \right| \lambda_i \tag{8}$$

Since for all $i \in [1, n] \cap \mathbb{N}$ $\lambda_i \geq 0$ by assumption and $\left|a_i^2\right| \geq 0$ by definition of $|\cdot|$, then $\langle Tx, x \rangle \geq 0$ for all $x \in V$ by generalisation of (8). □

Lemma 0.2

T is positive semi-definite if and only if there exists a linear transformation $S \in \text{Hom}(V, V)$ such that $T = S^*S$.

Proof.

Suppose first T is positive semi-definite.

Thus, $T = T^*$ and $\langle T(x), x \rangle \geq 0$ for all $x \in V$.

Since T is self-adjoint, then by the Spectral Theorem there is an orthonormal basis $\beta = \{v_1, \ldots, v_n\}$ of eigenvectors, with the corresponding eigenvalues $\lambda_1, \ldots, \lambda_n$.

Define a linear transformation S, $S \in \text{Hom}(V, V)$, so that $Sv_i = \sqrt{\lambda_i} v_i$. Since any linear transformation is defined by its action on a basis, S is well-defined.

By Lemma 0.1, any λ_i is real and nonnegative. Hence, by definition of S, all eigenvalues of S are real and nonnegative. Moreover, since β is a basis and also a set of all eigenvectors of S, then, by Lemma 0.1 again, T is self-adjoint. Therefore, by definition, S is positive semi-definite.

Note that for any $v_i \in \beta$ $S(Sv_i) = \lambda_i v_i = Tv_i$, by construction of S and since v_i is an eigenvector of T. Since $v_i \in \beta$, which is a basis of V, and T and S^2 are defined uniquely by its action on a basis, then $S^2 = T$.

Since S is positive-definite, $S = S^*$, and thus $T = S^*S$.

Suppose now there exists a linear transformation $S \in \text{Hom}(V, V)$ such that $T = S^*S$.

Therefore, $T^* = (S^*S)^* = S^*S = T$, and hence T is self-adjoint. By the Spectral Theorem there is an orthonormal basis $\beta = \{v_1, \ldots, v_n\}$ of V, consisting of eigenvectors of T, with the corresponding eigenvalues $\lambda_1, \ldots, \lambda_n$.

For any $v \in V$, consider $\langle Tv, v \rangle$:

$$\langle Tv, v \rangle = \langle S^*Sv, v \rangle \tag{9}$$

$$= \langle Sv, Sv \rangle \tag{10}$$

$$= \|Sv\| \geq 0 \tag{11}$$

Therefore, for all $v \in V$, $\langle Tv, v \rangle \geq 0$ and thus T is positive semi-definite. □

Question 0.3. Is it true that T is positive semi-definite if and only if there exists a linear transformation $S \in \text{Hom}(V, V)$ such that $T = S^2$?

Answer. From the proof of Lemma 0.2, it is true that if T is positive semi-definite, then there exists a linear transformation $S \in \text{Hom}(V, V)$ such that $T = S^2$.

However, suppose $T = \begin{pmatrix} 1 & -2 \\ 0 & 1 \end{pmatrix}$. It is easy to check that if $S = \begin{pmatrix} -1 & 1 \\ 0 & -1 \end{pmatrix}$, then $T = S^2$. However, since $T^* = \begin{pmatrix} 1 & 0 \\ -2 & 1 \end{pmatrix} \neq T$, then T is not self-adjoint and hence not positive semi-definite.