Maximization of Quadratic Forms for Points on the Unit Sphere. Let $\underset{(p\times p)}{\mathbf{B}}$ be a positive definite matrix with eigenvalues $\lambda_1 \ge \lambda_2 \ge \cdots \ge \lambda_p > 0$ and associated normalized eigenvectors $\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_p$. Then

$$\max_{\mathbf{x}\neq\mathbf{0}} \frac{\mathbf{x}'\mathbf{B}\mathbf{x}}{\mathbf{x}'\mathbf{x}} = \lambda_1 \qquad \text{attained when } \mathbf{x} = \mathbf{e}_1$$

$$\min_{\mathbf{x}\neq\mathbf{0}} \frac{\mathbf{x}'\mathbf{B}\mathbf{x}}{\mathbf{x}'\mathbf{x}} = \lambda_p \qquad \text{attained when } \mathbf{x} = \mathbf{e}_p \tag{2-51}$$

Moreover,

$$\max_{\mathbf{x}\perp\mathbf{e}_1,\ldots,\mathbf{e}_k} \frac{\mathbf{x}'\mathbf{B}\mathbf{x}}{\mathbf{x}'\mathbf{x}} = \lambda_{k+1} \quad \text{attained when } \mathbf{x} = \mathbf{e}_{k+1}, k = 1, 2, \ldots, p-1 \tag{2-52}$$

where the symbol $\perp$ is read "perpendicular to."

Proof. Let $\underset{(p\times p)}{\mathbf{P}}$ be the orthogonal matrix whose columns are the eigenvectors $\mathbf{e}_1, \mathbf{e}_2, \ldots, \mathbf{e}_p$ and $\mathbf{\Lambda}$ be the diagonal matrix with eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_p$ along the main diagonal. Let $\mathbf{B}^{1/2} = \mathbf{P}\mathbf{\Lambda}^{1/2}\mathbf{P}'$ [see (2-22)] and $\underset{(p\times 1)}{\mathbf{y}} = \underset{(p\times p)}{\mathbf{P}'}\underset{(p\times 1)}{\mathbf{x}}$. Consequently, $\mathbf{x} \neq \mathbf{0}$ implies $\mathbf{y} \neq \mathbf{0}$. Thus

$$\frac{\mathbf{x}'\mathbf{B}\mathbf{x}}{\mathbf{x}'\mathbf{x}} = \frac{\mathbf{x}'\mathbf{B}^{1/2}\mathbf{B}^{1/2}\mathbf{x}}{\mathbf{x}'\underbrace{\mathbf{P}\mathbf{P}'}_{\underset{(p\times p)}{\mathbf{I}}}\mathbf{x}} = \frac{\mathbf{x}'\mathbf{P}\mathbf{\Lambda}^{1/2}\mathbf{P}'\mathbf{P}\mathbf{\Lambda}^{1/2}\mathbf{P}'\mathbf{x}}{\mathbf{y}'\mathbf{y}} = \frac{\mathbf{y}'\mathbf{\Lambda}\mathbf{y}}{\mathbf{y}'\mathbf{y}} = \frac{\sum_{i=1}^{p}\lambda_i y_i^2}{\sum_{i=1}^{p} y_i^2} \le \lambda_1 \frac{\sum_{i=1}^{p} y_i^2}{\sum_{i=1}^{p} y_i^2} = \lambda_1 \tag{2-53}$$

Setting $\mathbf{x} = \mathbf{e}_1$ gives

$$\mathbf{y} = \mathbf{P}'\mathbf{e}_1 = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

since

$$\mathbf{e}_k'\mathbf{e}_1 = \begin{cases} 1 & k = 1 \\ 0 & k \neq 1 \end{cases}$$

For this choice of $\mathbf{x}$, $\mathbf{y}'\mathbf{\Lambda}\mathbf{y}/\mathbf{y}'\mathbf{y} = \lambda_1/1 = \lambda_1$, or

$$\frac{\mathbf{e}_1'\mathbf{B}\mathbf{e}_1}{\mathbf{e}_1'\mathbf{e}_1} = \mathbf{e}_1'\mathbf{B}\mathbf{e}_1 = \lambda_1 \tag{2-54}$$

A similar argument produces the second part of (2-51).

Now $\mathbf{x} = \mathbf{P}\mathbf{y} = y_1\mathbf{e}_1 + y_2\mathbf{e}_2 + \cdots + y_p\mathbf{e}_p$, so $\mathbf{x} \perp \mathbf{e}_1, \ldots, \mathbf{e}_k$ implies

$$0 = \mathbf{e}_i'\mathbf{x} = y_1\mathbf{e}_i'\mathbf{e}_1 + y_2\mathbf{e}_i'\mathbf{e}_2 + \cdots + y_p\mathbf{e}_i'\mathbf{e}_p = y_i, \quad i \le k$$

Therefore, for $\mathbf{x}$ perpendicular to the first k eigenvectors $\mathbf{e}_i$, the left-hand side of the inequality in (2-53) becomes

$$\frac{\mathbf{x}'\mathbf{B}\mathbf{x}}{\mathbf{x}'\mathbf{x}} = \frac{\sum_{i=k+1}^{p}\lambda_i y_i^2}{\sum_{i=k+1}^{p} y_i^2}$$

Taking $y_{k+1} = 1, y_{k+2} = \cdots = y_p = 0$ gives the asserted maximum. ■