设单位向量$\boldsymbol{x}$是实对称矩阵$\boldsymbol{A}$对应特征值$\boldsymbol{\lambda}$的特征向量, 单位向量$\boldsymbol{x}_0$是$\boldsymbol{x}$的一个$\mathcal{O}(\epsilon)$近似, 即$\boldsymbol{x}_0 = \boldsymbol{x} + \mathcal{O}(\epsilon)$. 定义$\mu_0 = \boldsymbol{x}_0^T \boldsymbol{A} \boldsymbol{x}_0$, 和$\boldsymbol{x}_1 = \boldsymbol{z}_1/||\boldsymbol{z}_1||_2$, 其中$\boldsymbol{z}_1$是方程组$(\boldsymbol{A} - \mu_0 \boldsymbol{I})\boldsymbol{z}_1 = \boldsymbol{x}_0$的解. 请给出$\mu_1 = \boldsymbol{x}_1^T \boldsymbol{A} \boldsymbol{x}_1$和特征值$\boldsymbol{\lambda}$的误差估计.

解: 设所求特征值为λ, 设$\boldsymbol{x}_0 = \rho \boldsymbol{x} + \boldsymbol{x}^{\perp}$, 其中$\|\boldsymbol{x}^{\perp}\|_2 = \mathcal{O}(\epsilon)$, $\rho^2 = 1 - \|\boldsymbol{x}^{\perp}\|_2^2 \leq 1$ (因为x_0是单位向量), 则由于$(\boldsymbol{A} - \mu_0 \boldsymbol{I})\boldsymbol{x} = (\lambda - \mu_0)\boldsymbol{x}$,

$$\boldsymbol{z}_1 = (\boldsymbol{A} - \mu_0 \boldsymbol{I})^{-1} \rho \boldsymbol{x} + (\boldsymbol{A} - \mu_0 \boldsymbol{I})^{-1} \boldsymbol{x}^{\perp} = \frac{\rho}{\lambda - \mu_0} \boldsymbol{x} + (\boldsymbol{A} - \mu_0 \boldsymbol{I})^{-1} \boldsymbol{x}^{\perp},$$

则

$$\begin{aligned}
||\boldsymbol{z}_1||_2^2 &= \frac{\rho^2}{(\lambda - \mu_0)^2} + \frac{2\rho}{\lambda - \mu_0} \boldsymbol{x}^T (\boldsymbol{A} - \mu_0 \boldsymbol{I})^{-1} \boldsymbol{x}^{\perp} + \left((\boldsymbol{A} - \mu_0 \boldsymbol{I})^{-1} \boldsymbol{x}^{\perp}\right)^T (\boldsymbol{A} - \mu_0 \boldsymbol{I})^{-1} \boldsymbol{x}^{\perp} \\
&= \frac{\rho^2}{(\lambda - \mu_0)^2} + \left((\boldsymbol{A} - \mu_0 \boldsymbol{I})^{-1} \boldsymbol{x}^{\perp}\right)^T (\boldsymbol{A} - \mu_0 \boldsymbol{I})^{-1} \boldsymbol{x}^{\perp}.
\end{aligned}$$

另外,

$$\begin{aligned}
\boldsymbol{z}_1^T \boldsymbol{A} \boldsymbol{z}_1 &= \frac{\lambda \rho}{\lambda - \mu_0} \boldsymbol{z}_1^T \boldsymbol{x} + \boldsymbol{z}_1^T \boldsymbol{A} (\boldsymbol{A} - \mu_0 \boldsymbol{I})^{-1} \boldsymbol{x}^{\perp} \\
&= \frac{\lambda \rho}{\lambda - \mu_0} \left(\frac{\rho}{\lambda - \mu_0} \boldsymbol{x} + (\boldsymbol{A} - \mu_0 \boldsymbol{I})^{-1} \boldsymbol{x}^{\perp} \right)^T \boldsymbol{x} \\
&+ \left(\frac{\rho}{\lambda - \mu_0} \boldsymbol{x} + (\boldsymbol{A} - \mu_0 \boldsymbol{I})^{-1} \boldsymbol{x}^{\perp} \right)^T \boldsymbol{A} (\boldsymbol{A} - \mu_0 \boldsymbol{I})^{-1} \boldsymbol{x}^{\perp} \\
&= \frac{\lambda \rho^2}{(\lambda - \mu_0)^2} + \left((\boldsymbol{A} - \mu_0 \boldsymbol{I})^{-1} \boldsymbol{x}^{\perp}\right)^T \boldsymbol{A} (\boldsymbol{A} - \mu_0 \boldsymbol{I})^{-1} \boldsymbol{x}^{\perp}.
\end{aligned}$$

记$\boldsymbol{y} := (\boldsymbol{A} - \mu_0 \boldsymbol{I})^{-1} \boldsymbol{x}^{\perp}$, 则

$$\mu_1 = \frac{\boldsymbol{z}_1^T \boldsymbol{A} \boldsymbol{z}_1}{||\boldsymbol{z}_1||_2^2} = \frac{\frac{\lambda \rho^2}{(\lambda - \mu_0)^2} + ||\boldsymbol{y}||_{\boldsymbol{A}}^2}{\frac{\rho^2}{(\lambda - \mu_0)^2} + ||\boldsymbol{y}||_2^2} = \frac{\lambda \rho^2 + (\lambda - \mu_0)^2 ||\boldsymbol{y}||_{\boldsymbol{A}}^2}{\rho^2 + (\lambda - \mu_0)^2 ||\boldsymbol{y}||_2^2}.$$

则

$$\mu_1 - \lambda = \frac{(\lambda - \mu_0)^2 (||\boldsymbol{y}||_{\boldsymbol{A}}^2 - \lambda ||\boldsymbol{y}||_2^2)}{\rho^2 + (\lambda - \mu_0)^2 ||\boldsymbol{y}||_2^2}.$$

设$\boldsymbol{x}_i$, $i = 2, \cdots, n$为$\boldsymbol{A}$与$\boldsymbol{x}$正交的单位特征向量，对应的特征值为λ_i, $i = 2, \cdots, n$. 于是存在组合系数c_i, $i = 2, \cdots, n$, 使得

$$\boldsymbol{x}^{\perp} = \sum_{i=2}^{n} c_i \boldsymbol{x}_i$$

且

$$\sum_{i=2}^{n} c_i^2 = \|\boldsymbol{x}^{\perp}\|_2^2 = \mathcal{O}(\epsilon^2).$$

这样

$$\boldsymbol{y} = (\boldsymbol{A} - \mu_0 I)^{-1}\boldsymbol{x}^{\perp} = \sum_{i=2}^{n} \frac{c_i \boldsymbol{x}_i}{\lambda_i - \mu_0},$$

$$\|\boldsymbol{y}\|_{\boldsymbol{A}}^2 = \sum_{i=2}^{n} \frac{c_i^2 \lambda_i}{(\lambda_i - \mu_0)^2}, \|\boldsymbol{y}\|_0^2 = \sum_{i=2}^{n} \frac{c_i^2}{(\lambda_i - \mu_0)^2}.$$

设$\lambda = \lambda_2 = \cdots = \lambda_\ell$, 但$\lambda_{\ell+1}, \cdots, \lambda_n \neq \lambda$, $\ell \leq n$. 于是

$$\begin{aligned}
\mu_1 - \lambda &= \frac{(\lambda - \mu_0)^2(\|\boldsymbol{y}\|_{\boldsymbol{A}}^2 - \lambda\|\boldsymbol{y}\|_2^2)}{\rho^2 + (\lambda - \mu_0)^2\|\boldsymbol{y}\|_2^2} \\
&= \frac{(\lambda - \mu_0)^2 \sum\limits_{i=\ell+1}^{n} c_i^2(\lambda_i - \lambda)/(\lambda_i - \mu_0)^2}{\rho^2 + \sum\limits_{i=2}^{\ell} c_i^2 + (\lambda - \mu_0)^2 \sum\limits_{i=\ell+1}^{n} c_i^2/(\lambda_i - \mu_0)^2}.
\end{aligned}$$

由于$\rho^2 + \|\boldsymbol{x}^{\perp}\|_2^2 = 1$, 得$1 - \rho^2 = \|\boldsymbol{x}^{\perp}\|_2^2 = \mathcal{O}(\epsilon^2)$. 因此，

$$\begin{aligned}
&\mu_0 - \lambda = \boldsymbol{x}_0^T \boldsymbol{A} \boldsymbol{x}_0 - \lambda \\
&= \rho^2 \boldsymbol{x}^T A \boldsymbol{x} + 2\rho \boldsymbol{x}^T A \boldsymbol{x}^{\perp} + (\boldsymbol{x}^{\perp})^T A \boldsymbol{x}^{\perp} - \lambda \\
&= \lambda(\rho^2 - 1) + (\boldsymbol{x}^{\perp})^T \boldsymbol{A} \boldsymbol{x}^{\perp} \\
&= (\boldsymbol{x}^{\perp})^T \boldsymbol{A} \boldsymbol{x}^{\perp} - \lambda \|\boldsymbol{x}^{\perp}\|_2^2 \\
&= \sum_{i=\ell+1}^{n} c_i^2(\lambda_i - \lambda) = \mathcal{O}(\epsilon^2).
\end{aligned}$$

代入前式，得

$$\mu_1 - \lambda = \mathcal{O}(\epsilon^6).$$

$\blacksquare$