Eigenvalue Perturbation Theory

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In this note we write the formal expression for the perturbation serie of an eigenvalue at any order.

1 Eigenvalue Perturbation Theory

Let $\lambda_1(t) \geq \lambda_2(t) \geq \cdots \geq \lambda_N(t)$ the eigenvalue of the symmetric matrix $A + tB$. We denote $\lambda_j = \lambda_j(0)$ to shorten the notation and assume that A is diagonal $A = \text{diag}(\lambda_1, \cdots, \lambda_N)$. Let $i \in \{1, \cdots, N\}$, we assume that at $t = 0$, the i-th eigenvalue is non degenerate : $\lambda_{i-1} > \lambda_i > \lambda_{i+1}$. Let $\lambda_i^{(k)}$ the $k-$term of the development in perturbation theory

$$\lambda_i(t) = \sum_{k=0}^{\infty} t^k \lambda_i^{(k)}.$$

We denote $f_{k,m}^{(m)}$ the $m-$th derivative of the function

$$f_{k,m}(z) := \sum_{\substack{1 \leq j_1, \cdots, j_k \leq N \\ |\{j_l = i\}| = m+1}} \frac{\prod_{l=1}^{k} B_{j_l j_{l+1}}}{\prod_{l \leq k, \lambda_{j_l} \neq \lambda_i} (z - \lambda_{j_l})} dz \tag{1}$$

where we identify $j_{k+1} = j_1$.

Theorem 1. *For $k \geq 2$, we have*

$$\lambda_i^{(k)} = \frac{1}{k} \sum_{m=0}^{k-2} \frac{1}{m!} f_{k,m}^{(m)}(\lambda_i)$$

In short to compute the expression of the $k - th$ order perturbation it is enough to

1. Draw all the paths of lenght k in $\{1, \cdots, N\}$ and at each step l multiply by $\frac{B_{j_l j_{l+1}}}{(z - \lambda_{j_l})}$.
2. In each expression, put the $\frac{1}{(z-\lambda_i)}$ aside and for each of these terms differentiate in z what is left.
3. Sum everything.

2 Proof of Theorem 1,

To prove Theorem 1, we start with the following lemma. Let $\epsilon > 0$ and $T > 0$ small enough so that $\forall t \in [-T, T]$,

$$\lambda_{i-1}(t) > \lambda_i(0) + \epsilon > \lambda_i(t) > \lambda_i(0) - \epsilon > \lambda_{i+1}(t)$$

Let $\mathcal{C}_\epsilon(i)$ the small circle in $\mathbb{C}$ around $\lambda_i(0)$ of radius that is the i-th eigenvalue.

Lemma 2. *For $k \geq 1$*

$$\lambda_i^{(k)} = \frac{1}{2i\pi k} \oint_{\mathcal{C}_\epsilon(i)} Tr([(z-A)^{-1}B]^k)dz.$$

Proof of Lemma 2. Here $\forall t \in [-T, T]$, $\lambda_i(t)$ stay inside the circle and the others eigenvalues stay outside. With the Cauchy formula we have

$$\lambda_i(t) = \frac{1}{2i\pi} \oint_{\mathcal{C}_\epsilon(i)} z\mathrm{Tr}((z - A - tB)^{-1})dz$$

We write down the development

$$\begin{aligned}(z - A - tB)^{-1} &= ((I - t(z-A)^{-1}B)^{-1}(z-A)^{-1} \\ &= \sum_{k=0}^{\infty} t^k [(z-A)^{-1}B]^k (z-A)^{-1}\end{aligned}$$

and we obtain

$$\lambda_i(t) = \sum_{k=0}^{\infty} t^k \frac{1}{2i\pi} \oint_{\mathcal{C}_\epsilon(i)} z\mathrm{Tr}([(z-A)^{-1}B]^k (z-A)^{-1})dz.$$

Remark that

$$\frac{d}{dz}\mathrm{Tr}([(z-A)^{-1}B]^k = -k\mathrm{Tr}([(z-A)^{-1}B]^k(z-A)^{-1}).$$

Therefore for $k \geq 1$

$$\begin{aligned}\lambda_i^{(k)} &= -\frac{1}{2i\pi k} \oint_{\mathcal{C}_\epsilon(i)} z\frac{d}{dz}\mathrm{Tr}([(z-A)^{-1}B]^k)dz \\ &= \frac{1}{2i\pi k} \oint_{\mathcal{C}_\epsilon(i)} \mathrm{Tr}([(z-A)^{-1}B]^k)dz\end{aligned}$$

□

Proof of Theorem 1. We use Lemma 2 with $A = \operatorname{diag}(\lambda_1, \cdots, \lambda_N)$ to obtain

$$
\begin{aligned}
\lambda_i^{(k)} &= \sum_{1 \le j_1, \cdots, j_k \le N} \frac{1}{2i\pi k} \oint_{\mathcal{C}_\epsilon(i)} \prod_{l=1}^{k} \frac{B_{j_l j_{l+1}}}{(z-\lambda_{j_l})} dz \\
&= \sum_{m=0}^{k-1} \frac{1}{2i\pi k} \oint_{\mathcal{C}_\epsilon(i)} \frac{1}{(z-\lambda_i)^{m+1}} \sum_{\substack{1 \le j_1, \cdots, j_k \le N \\ |\{j_l = i\}| = m+1}} \frac{\prod_{l=1}^{k} B_{j_l j_{l+1}}}{\prod_{l \le k, \lambda_{j_l} \ne \lambda_i} (z - \lambda_{j_l})} dz \\
&= \frac{1}{k} \sum_{m=0}^{k-1} \frac{1}{m!} f_{k,m}^{(m)}(\lambda_i)
\end{aligned}
$$

where we identify $j_{k+1} = j_1$ and denote $f_{k,m}^{(m)}$ the $m-$th derivative of the function $f_{k,m}$ as in (1). We remark that $f_{k,k-1} = B_{ii}^k$ so for $k \ge 2$, $f_{k,k-1}^{(k-1)}(z) = 0$ and then $\lambda_i^{(k)} = \frac{1}{k} \sum_{m=0}^{k-2} \frac{1}{m!} f_{k,m}^{(m)}(\lambda_i)$. □

3 Application of the formula : compute the first orders.r

We compute here the first value of this development. Here we denote $\sum$ for $\sum_{j \in \{1, \cdots, N\} \setminus \{i\}}$.

1. We have $f_{1,0}(z) = B_{ii}$ and then

$$\lambda_i^{(1)} = B_{ii}.$$

2. We have

$$f_{2,0}(z) = \sum_j \frac{B_{ji} B_{ij} + B_{ij} B_{ji}}{(z - \lambda_j)}$$

and therefore

$$\lambda_i^{(2)} = \sum_j \frac{B_{ij}^2}{(\lambda_i - \lambda_j)}.$$

3. We have

$$
\begin{aligned}
f_{3,0}(z) &= \sum_{j,l} \frac{B_{ij} B_{jl} B_{li} + B_{ji} B_{il} B_{lj} + B_{jl} B_{li} B_{lj}}{(z-\lambda_j)(z-\lambda_l)} \\
f_{3,1}(z) &= \sum_{j} \frac{B_{ij} B_{ji} B_{ii} + B_{ii} B_{ij} B_{ji} + B_{ji} B_{ii} B_{ij}}{(z-\lambda_j)}
\end{aligned}
$$

so we obtain

$$\lambda_i^{(3)} = \sum_{j,l} \frac{B_{ij} B_{jl} B_{li}}{(\lambda_i - \lambda_j)(\lambda_i - \lambda_l)} - \sum_j \frac{B_{ij} B_{ji} B_{ii}}{(\lambda_i - \lambda_j)^2}$$

4. We have

$$
\begin{aligned}
f_{4,0}(z) &= 4\sum_{j,k,l} \frac{B_{ij}B_{jk}B_{kl}B_{li}}{(z-\lambda_j)(z-\lambda_k)(z-\lambda_l)} \\
f_{4,1}(z) &= \sum_{j,k} \frac{4B_{ij}B_{jk}B_{ki}B_{ii} + 2B_{ij}B_{ji}B_{ik}B_{ki}}{(z-\lambda_j)(z-\lambda_k)} \\
f_{4,2}(z) &= \sum_{j} \frac{4B_{ij}B_{ji}B_{ii}B_{ii}}{(z-\lambda_j)}
\end{aligned}
$$

so we obtain

$$
\begin{aligned}
\lambda_i^{(4)} = &\sum_{j,k,l} \frac{B_{ij}B_{jk}B_{kl}B_{li}}{(\lambda_i-\lambda_j)(\lambda_i-\lambda_l)} - \sum_{j,k} \frac{2B_{ij}B_{jk}B_{ki}B_{ii} + B_{ij}B_{ji}B_{ik}B_{ki}}{(\lambda_i-\lambda_j)^2(\lambda_i-\lambda_k)} \\
&+ \sum_{j} \frac{B_{ij}B_{ji}B_{ii}B_{ii}}{(z-\lambda_j)^3}
\end{aligned}
$$