Perturbation Theory for Eigenvalue Problem

$(A+\varepsilon B)\vec{x}_i = \lambda_i \vec{x}_i$:

Unperturbed problem: $A\vec{e}_i = a_i \vec{e}_i$

Assuming a_i is non-degenerate use expansion:

$$\vec{x}_i(\varepsilon) = \vec{e}_i + \varepsilon \vec{x}_i^{(1)} + \varepsilon^2 \vec{x}_i^{(2)} + \cdots$$

$$\lambda_i(\varepsilon) = a_i + \varepsilon \lambda_i^{(1)} + \varepsilon^2 \lambda_i^{(2)} + \cdots$$

$$(A+\varepsilon B)(\vec{e}_i + \varepsilon \vec{x}_i^{(1)} + \varepsilon^2 \vec{x}_i^{(2)} + \cdots) = (a_i + \varepsilon\lambda_i^{(1)} + \varepsilon^2 \lambda_i^{(2)} + \cdots)(\vec{e}_i + \varepsilon \vec{x}_i^{(1)} + \varepsilon^2 \vec{x}_i^{(2)} + \cdots)$$

at ε^0: $A\vec{e}_i = a_i \vec{e}_i$ (correct choice of $\vec{x}_i^{(0)}, \lambda_i^{(0)}$)

ε^1: $A\vec{x}_i^{(1)} + B\vec{e}_i = a_i \vec{x}_i^{(1)} + \lambda_i^{(1)}\vec{e}_i$

ε^2: $A\vec{x}_i^{(2)} + B\vec{x}_i^{(1)} = a_i \vec{x}_i^{(2)} + \lambda_i^{(1)}\vec{x}_i^{(1)} + \lambda_i^{(2)}\vec{e}_i$

. . .

First order perturbations

Define *left* eigenvectors: $\vec{f}_i A = a_i \vec{f}_i$

Note: $\vec{f}_j \cdot \vec{e}_i = 0$, $\forall j \neq i$ => Normalize: $(\vec{f}_i \cdot \vec{e}_i) = 1$

Note: For A - Hermitian (Symmetric) $\vec{f}_i = \vec{e}_i$

$$\vec{f}_j \cdot (A\vec{x}_i^{(1)} + B\vec{e}_i) = \vec{f}_j \cdot (a_i \vec{x}_i^{(1)} + \lambda_i^{(1)}\vec{e}_i)$$

$$\Rightarrow \quad a_j(\vec{f}_j \cdot \vec{x}_i^{(1)}) + (\vec{f}_j \cdot B\vec{e}_i) = a_i(\vec{f}_j \cdot \vec{x}_i^{(1)}) + \lambda_i^{(1)}\delta_{ij}$$

Solve with respect to $\lambda_i^{(1)}$ for $j = i$: $\boxed{\lambda_i^{(1)} = (\vec{f}_i \cdot B\vec{e}_i)}$

Let $\vec{x}_i^{(1)} = \sum_j c_j^{(1)} \vec{e}_j$ $\Longrightarrow$ $(\vec{f}_j \cdot \vec{x}_i^{(1)}) = c_j^{(1)}$

Solve with respect to $c_j^{(1)}$ for $j \neq i$: $c_j^{(1)} = \dfrac{(\vec{f}_j \cdot B\vec{e}_i)}{a_i - a_j}$

Finally obtain $\vec{x}_i^{(1)} = c_i^{(1)}\vec{e}_i + \sum_{j\neq i} \frac{(\vec{f}_j \cdot B\vec{e}_i)}{a_i - a_j}\vec{e}_j$

Note: perturbation expansion does not fix the value of c_i^{1}!

To make the choice unique can require $(\vec{f}_i \cdot \vec{x}_i^{(1)}) = c_i^{(1)} = 0$

Second order perturbations

$$\vec{f}_j \cdot (A\vec{x}_i^{(2)} + B\vec{x}_i^{(1)}) = \vec{f}_j \cdot (a_i\vec{x}_i^{(2)} + \lambda_i^{(1)}\vec{x}_i^{(1)} + \lambda_i^{(2)}\vec{e}_i)$$

$$\Rightarrow \quad (a_j - a_i)(\vec{f}_j \cdot \vec{x}_i^{(2)}) + (\vec{f}_j \cdot B\vec{x}_i^{(1)}) = \lambda_i^{(1)}(\vec{f}_j \cdot \vec{x}_i^{(1)}) + \lambda_i^{(2)}\delta_{ij}$$

For $j = i$ obtain

$$\boxed{\lambda_i^{(2)} = (\vec{f}_i \cdot B\vec{x}_i^{(1)}) = \sum_{j\neq i} \frac{(\vec{f}_j \cdot B\vec{e}_i)(\vec{f}_i \cdot B\vec{e}_j)}{a_i - a_j}}$$

For $j \neq i$ obtain $\left(\vec{x}_i^{(2)} = \sum_j c_j^{(2)} e_j\right)$:

$$(a_i - a_j)\, c_j^{(2)} = -(\vec{f}_j \cdot B\vec{x}_i^{(1)}) + \lambda_i^{(1)}(\vec{f}_j \cdot x_i^{(1)})$$

so that

$$\vec{x}_i^{(2)} = c_i^{(2)}\vec{e}_i - \sum_{\substack{j\neq i \\ k\neq i,j}} \frac{(\vec{f}_k \cdot B\vec{e}_i)(\vec{f}_j \cdot B\vec{e}_k)}{(a_i - a_k)(a_i - a_j)}\vec{e}_j$$

Note: $c_i^{(2)}$ is again undetermined (neither will be $c_i^{(3)}, c_i^{(4)}, \ldots$)!

Example:

$$\begin{pmatrix} E_1 & \varepsilon \\ \varepsilon & E_2 \end{pmatrix} = \underbrace{\begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix}}_{A} + \varepsilon \underbrace{\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}}_{B}$$

A-symmetric $\Rightarrow$ $\vec{e}_1 = \vec{f}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $\vec{e}_2 = \vec{f}_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$: $a_1 = E_1$, $a_2 = E_2$.

First order:

$$\lambda_1^{(1)} = \vec{e}_1 \cdot B\vec{e}_1 = (1\ 0)\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0$$

$$x_1^{(1)} = \frac{\vec{e}_2 \cdot B\vec{e}_1}{E_1 - E_2}\vec{e}_2 = \frac{1}{\Delta E}\vec{e}_2 \quad \text{(can add a multiple of } \vec{e}_1\text{)}$$

Similarly $\lambda_2^{(1)}$, $\vec{x}_2^{(1)}$: swap $1 \leftrightarrow 2$

Second order: $\lambda_1^{(2)} = \dfrac{(\vec{e}_2 \cdot B\vec{e}_1)(\vec{e}_1 \cdot B\vec{e}_2)}{E_1 - E_2} = \dfrac{1}{\Delta E}$

$\vec{x}_1^{(2)} = 0$ (there is no index $k \neq 1,2$: Generic feature of 2×2 matrices – 2^{nd} order correction $\vec{x}_i^{(2)} = 0$!)

similarly $\lambda_2^{(2)}, \vec{x}_2^{(2)}$: swap $1 \Leftrightarrow 2$

Collecting everything together:

$$\lambda_1 = E_1 + \frac{\varepsilon^2}{\Delta E} + O(\varepsilon^3)\,, \quad \vec{x}_1 = \begin{pmatrix}1\\0\end{pmatrix} + \frac{\varepsilon}{\Delta E}\begin{pmatrix}0\\1\end{pmatrix} + O(\varepsilon^3)$$

Exact result: $\det\begin{pmatrix} E_1-\lambda & \varepsilon \\ \varepsilon & E_2-\lambda\end{pmatrix} = (E_1-\lambda)(E_2-\lambda) - \varepsilon^2 = 0$

$$\lambda^2 - (E_1+E_2)\lambda + E_1E_2 - \varepsilon^2 = 0$$

$$\lambda_{1,2} = \frac{E_1+E_2 \pm \sqrt{(E_1+E_2)^2 - 4(E_1E_2-\varepsilon^2)}}{2} =$$

$$= \frac{E_1+E_2 \pm \sqrt{(E_1-E_2)^2 + 4\varepsilon^2}}{2} =$$

$$= \frac{E_1+E_2 \pm |E_1-E_2|\left(1 + 2\frac{\varepsilon^2}{\Delta E} + \dots\right)}{2} = \left[\begin{array}{l} E_1 + \frac{\varepsilon^2}{\Delta E} + \dots \\ E_2 - \frac{\varepsilon^2}{\Delta E} + \dots \end{array}\right.$$

Example: Hydrogen atom in "strong" electric field:

$$\left[-\frac{\hbar^2}{2m}\nabla^2 - \frac{e^2}{r} + e\mathcal{E}z + \underset{\nwarrow \text{ polarization Coeff.}}{\alpha} e\mathcal{E}^2 z^2\right]\Psi = E\,\Psi$$

For instanse, 2p level $\Psi_{2p} = C(x \pm iy)e^{-r/2a_0}\,, \quad C^{-2} = 64\pi a_0^5$

has unperturbed energy $E_{2p} = -\dfrac{e^2}{8a_0}\,, \quad a_0^{-1} = \dfrac{2me^2}{\hbar^2}$

$$\Delta E_{2p} = \langle \Psi_{2p} | e\mathcal{E}z + \alpha e\mathcal{E}^2 z^2 | \Psi_{2p}\rangle = \int \Psi_{2p}^*(\vec{r})\Psi_{2p}(\vec{r})(e\mathcal{E}z + \alpha e\mathcal{E}^2z^2)\,d\vec{r}$$

$$= \int c^2 e^{-r/a_0}(x^2+y^2)(\overset{0\ (odd)}{e\mathcal{E}z} + \alpha e\mathcal{E}^2z^2)\,d\Omega\, r^2dr$$

$$= \frac{\alpha e\mathcal{E}^2}{64\pi a_0^5}\int r^2dr\, e^{-r/a_0}\int (r^2 - z^2)z^2 d\Omega = (6\alpha e a_0^2)\mathcal{E}^2$$

$$\Rightarrow E = -\frac{e^2}{8a_0} + \underset{\uparrow}{6\alpha a_0^2\mathcal{E}^2}$$

1^{st} order correction, which is quadratic in the field $\mathcal{E}$

Degenerate perturbation theory

If a_1 is degenerate $a_1 = a_2 = \cdots = a_n$, we have to perturb around a general eigenvector:

$$\vec{x}_1 = \sum_{k=1}^{n} \alpha_k \vec{e}_k + \varepsilon \vec{x}_1^{(1)} + \cdots$$

$$\lambda_1 = a_1 + \varepsilon \lambda_1^{(1)} + \cdots$$

Substitution into $(A+\varepsilon B)\vec{x}_1 = \lambda_1 \vec{x}_1$ gives

at order ε: $\quad (A-a)\vec{x}_1 = \lambda_1^{(1)} \sum_{k=1}^{n} \alpha_k e_k - \sum_{k=1}^{n} \alpha_k B \vec{e}_k$

Multiplying on the left by left eigenvectors $\vec{f}_k$, $k=1,\dots,n$ obtain a system of n equations for λ_1:

$$\alpha_k \lambda_1^{(1)} = \sum_{i=1}^{n} \alpha_i \underbrace{(\vec{f}_k \cdot B \vec{e}_i)}_{\tilde{B}_{ki}} \Rightarrow \tilde{B}\vec{\alpha} = \lambda_1^{(1)} \vec{\alpha}\ , \quad \vec{\alpha} = (\alpha_1, \dots, \alpha_n)$$

Nontrivial solutions $\vec{\alpha} \neq 0$ only exist if $\lambda_1^{(1)}$ is an eigenvalue of $\tilde{B}$.

Secular equation: $\quad \det(\tilde{B} - \lambda_1^{(1)} \mathbb{I}) = 0$ gives 1st order perturbations

Non-diagonalizable matrices

If A cannot be diagonalized, find generalized eigenvectors:

$$\left.\begin{aligned} A\vec{e}_1 &= a\vec{e}_1 \\ A\vec{e}_2 &= a\vec{e}_2 + \vec{e}_1 \\ &\cdots \\ A\vec{e}_n &= a\vec{e}_n + \vec{e}_{n-1} \end{aligned}\right\} \quad \text{A is in Jordan normal form in the basis of } \vec{e}_1, \vec{e}_2, \dots, \vec{e}_n$$

In this case, perturbation expansion in powers of $\varepsilon^{1/k}$ is needed, for some integer $k \leq n$:

$$\vec{x}(\varepsilon) = \vec{e}_1 + \varepsilon^{1/k} \alpha_2 \vec{e}_2 + \varepsilon^{2/k} \alpha_3 \vec{e}_3 + \cdots + \varepsilon^{(k-1)/k} \alpha_k \vec{e}_k$$

$$\lambda(\varepsilon) = a + \varepsilon^{1/k} \lambda_1 + \lambda^{2/k} \lambda_2 + \cdots$$

Example: $y'' - \lambda y + \varepsilon y^k = 0$, $y(0) = y(\pi)$

Find eigenvalues $\lambda(\varepsilon)$ up to 1st order

Rewrite as $\underbrace{\frac{d^2}{dx^2} y}_{Ay} + \underbrace{\varepsilon y^k}_{B(y)} = \lambda y$

Note: the formulas don't change if we replace

$$\sum_i \alpha_i B \vec{e}_i \longrightarrow B\left(\sum_i \alpha_i \vec{e}_i\right)$$

0th order eigenvalues & eigenvectors $\Big\}$ $y'' = \lambda y$ & B.C. $\Rightarrow y_n^{(0)} = \frac{1}{\sqrt{\pi}} e^{inx}$

$\lambda_n^{(0)} = -n^2$

Degenerate problem: $\lambda_n = \lambda_{-n}$

$$y_n = \alpha_+ y_n^{(0)} + \alpha_- y_{-n}^{(0)} + \varepsilon y_n^{(1)} + \dots$$
$$\lambda_n = \lambda_n^{(0)} + \varepsilon \lambda_n^{(1)} + \dots$$

Note: left & right e-vect. are the same (you'll have to trust this)

$$\int y_{\pm n}^{(0)}(x)^* \cdot B(\alpha_- y_{-n}^{(0)}(x) + \alpha_+ y_{+n}^{(0)}(x))\, dx = \alpha_\pm \lambda_n^{(1)}$$

k = 1: $B(y) = y \Rightarrow \int = \alpha_\pm = \alpha_\pm \lambda_n^{(1)} \Rightarrow \lambda_n^{(1)} = 1$

Exactly what we expect: $\lambda_n = -n^2 + \varepsilon + \dots$, $y_n = \alpha_+ y_n^{(0)} + \alpha_- y_{-n}^{(0)} + \dots$

k = 2: $B(\alpha_+ y_+ + \alpha_- y_-) = \underbrace{\alpha_+^2 y_+^2}_{e^{2inx}} + \underbrace{2\alpha_+\alpha_- y_+ y_-}_{e^{i0}} + \underbrace{\alpha_-^2 y_-^2}_{e^{-2inx}}$

$\int = 0 \Rightarrow \lambda_n^{(1)} = 0$

$\lambda_n = -n^2 + 0 \cdot \varepsilon + \dots$, $y_n = \alpha_+ y_n^{(0)} + \alpha_- y_{-n}^{(0)} + \dots$

k = 3: $B(\alpha_+ y_+ + \alpha_- y_-) = \underbrace{\alpha_+^3 y_+^3}_{e^{3inx}} + \underbrace{3\alpha_+^2 \alpha_- y_+^2 y_-}_{e^{inx}} + \underbrace{3\alpha_+ \alpha_-^2 y_+ y_-^2}_{e^{-inx}} + \underbrace{\alpha_-^3 y_-^3}_{e^{-3inx}}$

$\int = 3\alpha_\pm^2 \alpha_\mp = \alpha_\pm \lambda_n^{(1)} \Rightarrow 3\alpha_+\alpha_- = \lambda_n^{(1)}$

$y_n = \alpha_- y_{-n}^{(0)} + \alpha_+ y_n^{(0)} + \dots$, $\lambda_n = -n^2 + 3\varepsilon\alpha_+\alpha_- + \dots$

Perturbation Theory for Degenerate Matrices

$$(A+\varepsilon B)\vec{x} = \lambda\vec{x}$$

$$\left.\begin{aligned}\lambda_i &= \lambda_i^{(0)} + \varepsilon\lambda_i^{(1)} + \cdots \\ \vec{x}_i &= \vec{x}_i^{(0)} + \varepsilon\vec{x}_i^{(1)} + \cdots\end{aligned}\right\} \begin{aligned}&(A+\varepsilon B)(\vec{x}_i^{(0)} + \varepsilon\vec{x}_i^{(1)} + \cdots) = \\ &= (\lambda_i^{(0)} + \varepsilon\lambda_i^{(1)} + \cdots)(\vec{x}_i^{(0)} + \varepsilon\vec{x}_i^{(1)} + \cdots)\end{aligned}$$

ε^0: $A\vec{x}_i^{(0)} = \lambda_i^{(0)}\vec{x}_i^{(0)}$

$\Rightarrow \lambda_i^{(0)} = a_i$ – eigenvalue of A, $\vec{x}_i^{(0)}$ – some eigenvector, which corresponds to a_i

We have not determined $\vec{x}_i^{(0)}$, if $\lambda_i^{(0)}$ is degenerate.

If $\lambda_i^{(0)}$ is n-times degenerate, $\vec{x}_i^{(0)} = \alpha_1^i\vec{e}_1 + \alpha_2^i\vec{e}_2 + \cdots \alpha_n^i\vec{e}_n$

Coefficients α_i are not determined by 0th order equations, they are determined by higher order equations!

ε^1: $A\vec{x}_i^{(1)} + B\vec{x}_i^{(0)} = \underset{\overset{\shortparallel}{a_i}}{\lambda_i^{(0)}}\vec{x}_i^{(1)} + \lambda_i^{(1)}\vec{x}_i^{(0)}$

Multiply by $\vec{f}_j$ on the left: $a_j(\vec{f}_j\cdot\vec{x}_i^{(1)}) + (\vec{f}_j\cdot B\vec{x}_i^{(0)}) =$
$= a_i(\vec{f}_j\cdot\vec{x}_i^{(1)}) + \lambda_i^{(1)}\vec{x}_i^{(0)}$

a) $j = 1,\dots,n$ $\rightarrow$ n equations for eigenvalue correction $\lambda_i^{(1)}$

b) $j \neq n+1,\dots,N$ $\Rightarrow$ N-n equations for eigenvector correction $\vec{x}_i^{(1)}$

a) $(\vec{f}_j\cdot B\vec{x}_i^{(0)}) = \sum\limits_{k=1}^{n}\alpha_k^i\underbrace{(\vec{f}_j\cdot B\vec{e}_k)}_{\tilde{B}_{jk}} = \lambda_i^{(1)}\sum\limits_{k=1}^{n}\alpha_k^i\underbrace{(\vec{f}_j\cdot\vec{e}_k)}_{\delta_{jk}} \Rightarrow \tilde{B}\vec{\alpha}^i = \lambda_i^{(1)}\vec{\alpha}^i$

If $\tilde{B}$ is non-degenerate, this eigenproblem determines both $\lambda_i^{(1)}$ (1st order term in eigenvalue expansion) and $\vec{\alpha}^i = (\alpha_1^i,\dots,\alpha_n^i)$ (0th order term in eigenvector expansion)

If $\tilde{B}$ is also degenerate, α_k^i might (or might not be) determined by higher orders of pert. theory

Example: $A = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, $B = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$

$\vec{f}_1 = \vec{e}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, $\vec{f}_2 = \vec{e}_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$, $\lambda^{(0)}_{1,2} = 1$

$\vec{x}^{(0)}_i = \alpha^i_1 \vec{e}_1 + \alpha^i_2 \vec{e}_2$; $\tilde{B}_{jk} = \vec{f}_j \circ B \vec{e}_k = \delta_{jk} = B$ -degenerate!

$\Rightarrow \lambda^{(1)}_i = 1$, $\alpha^i_{1,2}$ – arbitrary

(Solve exactly: $\lambda_{1,2} = 1 + \varepsilon$, $\vec{x}_i = \alpha^i_1 \vec{e}_1 + \alpha^i_2 \vec{e}_2$, $\forall \alpha^i_{1,2}$)

Example: $A = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$, $B = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$

$\tilde{B}_{jk} = \vec{f}_j \cdot B \vec{e}_k = B_{jk} \Rightarrow \lambda^{(1)2}_i - 1 = 0 \Rightarrow \lambda^{(1)}_i = \pm 1$ – non-degen.!

$\lambda^{(1)}_i = +1$: $\vec{\alpha} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \Rightarrow \vec{x}^{(0)}_i = \vec{e}_1 + \vec{e}_2 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

$\lambda^{(1)}_i = -1$: $\vec{\alpha} = \begin{pmatrix} 1 \\ -1 \end{pmatrix} \rightarrow \vec{x}^{(0)}_i = \vec{e}_1 - \vec{e}_2 = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$