

Perturbation Theory



1. Conventional nondegenerate perturbation theory

Consider a general eigenvalue problem

$$(1,1) \quad Lu = \lambda u$$

Where L can be a regular matrix or a linear differential operator, and u is the eigenvector.

It is well known that for any regular linear operator has a set of mutual orthogonal eigenvectors u_j that form a base for the space of functions. Mutual orthogonal means that $u_i u_j = 0$, for $i \neq j$

If u_1, u_2, u_3, \dots is an orthonormal, $u_j^2 = 1$ base of eigenvector the for (almost) any function ψ , we have:

$$\psi = a_1 u_1 + a_2 u_2 + a_3 u_3 + \dots$$

The j 'th term is found by taking the dot product with u_j , which gives: $a_j = u_j \cdot \psi / u_j^2 = u_j \cdot \psi$, since $u_i u_j = 0$, for $i \neq j$, and $u_j^2 = 1$

Suppose we have a differential operator L^0 , where the eigenvalues λ_n^0 and eigenfunctions u_n^0 are known, and we have an operator L that is only slightly different from an operator L_0 .

We then have the two equations:

$$(1,2) \quad L^0 u_n^0 = \lambda_n^0 u_n^0 \quad \text{and} \quad Lu = \lambda u$$

We wish to find an approximate solution to the second equation. We put

$$(1,3) \quad L = L^0 + Q,$$

where Q is supposed to be "small" compared to L . And let us assume that there exists a number δ less than one that in some manner represent the order of magnitude of $|Q/L|$

Then we assume that the eigenvalue λ , may be written as a series:

$$(1,4) \quad \lambda_n = \lambda_n^0 + \lambda_n^{(1)} + \lambda_n^{(2)} + \dots$$

The upper index indicate the order of the approximation, like 1, δ , δ^2

And the eigenfunctions may have a series expansion:

$$(1,5) \quad u_n = u_n^0 + \sum a_{mn}^{(1)} u_m^0 + \sum a_{mn}^{(2)} u_m^0 + \dots$$

Notice that u_n^0 is omitted from the sums,

Where again the upper index indicate the order of approximation δ , δ^2

We then substitute (1,4) and (1,5) into (1,3).

$$(1,6) \quad (L^0 + Q)(u_n^0 + \sum a_{mn}^{(1)}u_m^0 + \sum a_{mn}^{(2)}u_m^0) = (\lambda_n^0 + \lambda_n^{(1)} + \lambda_n^{(2)} + \dots)(u_n^0 + \sum a_{mn}^{(1)}u_m^0 + \sum a_{mn}^{(2)}u_m^0)$$

The first order terms give:

From our suppositions we have $L^0u_n^0 = \lambda_n^0u_n^0$, so we are left with:

$$(1.7) \quad Qu_n^0 + L^0(\sum a_{mn}^{(1)}u_m^0 + \sum a_{mn}^{(2)}u_m^0) = (\lambda_n^{(1)} + \lambda_n^{(2)} + \dots)(u_n^0 + \sum a_{mn}^{(1)}u_m^0 + \sum a_{mn}^{(2)}u_m^0)$$

When we evaluate the expression after doing the operation with L^0 , we obtain

$$Qu_n^0 + \sum a_{mn}^{(1)}\lambda_m^0u_m^0 + \sum a_{mn}^{(2)}\lambda_m^1u_m^0 + \dots = (\lambda_n^{(0)} + \lambda_n^{(1)} + \lambda_n^{(2)} + \dots)(u_n^0 + \sum a_{mn}^{(1)}u_m^0 + \sum a_{mn}^{(2)}u_m^0 + \dots)$$

Keeping only the first order term we find:

$$(1.8) \quad Qu_n^0 + \sum a_{mn}^{(1)}\lambda_m^0u_m^0 = \lambda_n^{(0)}u_n^0 + \lambda_n^{(0)}\sum a_{mn}^{(1)}u_m^0$$

If we dot both sides with u_n^0 we obtain, since $u_n^0 \cdot u_m^0 = 0$ for $n \neq m$

$$(1.9) \quad u_n^0 \cdot Qu_n^0 + u_n^0 \cdot \sum a_{mn}^{(1)}\lambda_m^0u_m^0 = \lambda_n^{(0)}u_n^0 + \lambda_n^{(0)}\sum a_{mn}^{(1)}u_m^0$$

All the dot products $u_n^0 \cdot u_m^0 = 0$ for $n \neq m$, and we are left with.

$$(1.10) \quad u_n^0 \cdot Qu_n^0 = \lambda_n^{(1)}$$

This is a very simple result. The first order correction to the eigenvalue can then be written as

$$\lambda_n^{(1)} = u_n^0 \cdot Qu_n^0 + O(Q^2)$$

Where “O” is read order of. To Find the first order corrected eigenvector, we dot the first order equation (1.8) with u_p^0 , $p \neq n$

$$u_p^0 \cdot Qu_n^0 + u_p^0 \cdot \sum a_{mn}^{(1)}\lambda_m^0u_m^0 = u_p^0 \cdot \lambda_n^{(0)}u_n^0 + u_p^0 \cdot \lambda_n^{(0)}\sum a_{mn}^{(1)}u_m^0$$

Which gives

$$u_p^0 \cdot Qu_n^0 + u_p^0 \cdot \sum a_{mn}^{(1)}\lambda_m^0u_m^0 = u_p^0 \cdot \lambda_n^{(0)}u_n^0 + u_p^0 \cdot \lambda_n^{(0)}\sum a_{mn}^{(1)}u_m^0$$

$$u_p^0 \cdot Qu_n^0 + a_{pn}^{(1)}\lambda_p^0 = \lambda_n^{(0)}a_{pn}^{(1)} \Leftrightarrow$$

$$u_p^0 \cdot Qu_n^0 = (\lambda_n^0 - \lambda_p^{(0)})a_{pn}^{(1)} \Leftrightarrow \text{Assuming that } \lambda_n^0 \neq \lambda_p^{(0)}$$

$$a_{pn}^{(1)} = \frac{u_p^0 \cdot Qu_n^0}{\lambda_n^0 - \lambda_p^{(0)}}$$

We can see from (1,9) and (1.10) that the perturbation Q may be considered small the numbers

$u_p^0 Q u_n^0$ are considered small compared to $\lambda_n^0 - \lambda_p^{(0)}$.

(1.11) Mathematical example.

Let there be given a matrix operator $L = \begin{pmatrix} 2 + \varepsilon & 1 - \varepsilon \\ 1 - \varepsilon & 2 + 2\varepsilon \end{pmatrix}$ where $\varepsilon \ll 1$, and

$$L^0 = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \quad \text{and therefore } Q = \varepsilon \begin{pmatrix} 1 & -1 \\ -1 & 2 \end{pmatrix}$$

The eigenvalues λ_1^0, λ_2^0 , are given by the determinant:

$$\begin{vmatrix} 2 - \lambda & 1 \\ 1 & 2 - \lambda \end{vmatrix} = 0 \Leftrightarrow (2 - \lambda)^2 - 1 = 0 \Leftrightarrow \lambda = 1 \vee \lambda = 3$$

This correspond to the eigenvectors: $\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} u_1^{(1)} \\ u_2^{(1)} \end{pmatrix} = \begin{pmatrix} u_1^{(1)} \\ u_2^{(1)} \end{pmatrix}$ and $\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} u_1^{(2)} \\ u_2^{(2)} \end{pmatrix} = 3 \begin{pmatrix} u_1^{(2)} \\ u_2^{(2)} \end{pmatrix}$

$$2u_1^{(1)} + u_2^{(1)} = u_1^{(1)} \quad \wedge \quad u_1^{(1)} + 2u_2^{(1)} = u_2^{(1)} \quad \vee \quad 2u_1^{(2)} + u_2^{(2)} = 3u_2^{(2)} \quad \wedge \quad u_1^{(2)} + 2u_2^{(2)} = 3u_2^{(2)}$$

$$u_1^{(1)} + u_2^{(1)} = 0 \quad \wedge \quad u_1^{(1)} + u_2^{(1)} = 0 \quad \vee \quad 2u_1^{(2)} - 2u_2^{(2)} = 0 \quad \wedge \quad u_1^{(2)} - u_2^{(2)} = 0$$

They have the solution (1,-1) and (1,1) and normalized:

$$\text{From the general formalism, we get: } \begin{pmatrix} u_1^{(1)} \\ u_2^{(1)} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} u_1^{(2)} \\ u_2^{(2)} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

Then by the general formalism:

$$\lambda_1^{(1)} = \frac{1}{\sqrt{2}} (1 \quad -1) \varepsilon \begin{pmatrix} 1 & -1 \\ -1 & 2 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{\varepsilon}{2} (2 \quad -3) \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{5}{2} \varepsilon$$

$$\lambda_2^{(1)} = \frac{1}{\sqrt{2}} (1 \quad 1) \varepsilon \begin{pmatrix} 1 & -1 \\ -1 & 2 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{\varepsilon}{2} (0 \quad 1) \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{1}{2} \varepsilon$$

So that

$$\lambda_1 = 3 + \frac{5}{2} \varepsilon + \dots \qquad \lambda_2 = 1 + \frac{1}{2} \varepsilon + \dots$$

Also

$$a_{21}^{(1)} = \frac{u_2 Q u_1}{\lambda_2^0 - \lambda_1^0} = \frac{\frac{1}{\sqrt{2}}(1 \ 1)\varepsilon \begin{pmatrix} 1 & -1 \\ -1 & 2 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}}{3-1} = -\frac{\varepsilon}{4}$$

$$a_{12}^{(2)} = \frac{u_1 Q u_2}{\lambda_1^0 - \lambda_2^0} = \frac{\frac{1}{\sqrt{2}}(1 \ -1)\varepsilon \begin{pmatrix} 1 & -1 \\ -1 & 2 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}}{1-3} = \frac{\varepsilon}{4}$$

$$u_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} - \frac{\varepsilon}{4} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \approx \frac{1}{\sqrt{2}} \begin{pmatrix} 1 - \frac{\varepsilon}{4} \\ 1 + \frac{\varepsilon}{4} \end{pmatrix}$$

$$u_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix} + \frac{\varepsilon}{4} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \approx \frac{1}{\sqrt{2}} \begin{pmatrix} 1 + \frac{\varepsilon}{4} \\ -1 + \frac{\varepsilon}{4} \end{pmatrix}$$

Reference: Mathews and Walker Mathematical Methods of Physics