Non-degenerate Perturbation Theory

Given an operator $\mathcal{A}$ such that

$$\mathcal{A} = \mathcal{A}^{(0)} + \epsilon \mathcal{A}^{(1)}$$

where $\mathcal{A}^{(0)}$ and $\mathcal{A}^{(1)}$ are both Hermitian, we wish to find the approximate eigenvectors and eigenvalues of $\mathcal{A}$:

$$\mathcal{A} x_i = \lambda_i \, x_i$$

given that we know the set of eigenvectors and eigenvalues of $\mathcal{A}^{(0)}$, that is, $\mathcal{A}|_{\epsilon=0}$.

$$\mathcal{A}^{(0)} x_i^{(0)} = \lambda_i^{(0)} x_i^{(0)}.$$

To do so we seek a power series solution of the form

$$\begin{aligned} x_i &= x_i^{(0)} + \epsilon \, x_i^{(1)} + \epsilon^2 \, x_i^{(2)} \ldots \\ \lambda_i &= \lambda_i^{(0)} + \epsilon \, \lambda_i^{(1)} + \epsilon^2 \, \lambda_i^{(2)} \ldots \end{aligned}$$

The first order correction to the eigenvalue is:

$$\lambda_i^{(1)} = \left(x_i^{(0)} \middle| \, \mathcal{A}^{(1)} x_i^{(0)} \right)$$

The first order correction to the eigenvector is:

$$x_i^{(1)} = \sum\nolimits_{k \neq i} \frac{\left(x_k^{(0)} \middle| \, \mathcal{A}^{(1)} x_n^{(0)} \right)}{\lambda_i^{(0)} - \lambda_k^{(0)}} \, x_k^{(0)}$$

The second order correction to the eigenvalue is:

$$\begin{aligned} \lambda_i^{(2)} &= \left(x_i^{(0)} \middle| \, \mathcal{A}^{(1)} x_i^{(1)} \right) \\ &= \sum_{k \neq i} \frac{\left| \left(x_k^{(0)} \middle| \, \mathcal{A}^{(1)} x_i^{(0)} \right) \right|^2}{\lambda_i^{(0)} - \lambda_k^{(0)}} \end{aligned}$$