COLLEGE OF ARTS AND SCIENCES
HOMER L. DODGE
DEPARTMENT OF PHYSICS AND ASTRONOMY
The UNIVERSITY of OKLAHOMA

Math Methods in Physics

PHYS 5013 HOMEWORK ASSIGNMENT #9

PROBLEMS: {1, 2, 3, 4}

Due: November 15, 2021 By 11:59 PM

STUDENT
Taylor Larrechea

PROFESSOR
Dr. Kieran Mullen

Problem 1:

Non-Degenerate Perturbation Theory: Consider the matrix

$$\mathcal{A} = \mathcal{A}_0 + \epsilon \mathcal{A}_1$$

where

$$\mathcal{A}_0 = \begin{pmatrix} -2 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -2 \end{pmatrix}$$

and

$$\mathcal{A}_1 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}.$$

(a) The matrix $\mathcal{A}$ has eigenvalues λ_i with eigenvectors x_i so that

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

Solve for the eigenvalues and normalized eigenvectors of $\mathcal{A}_0$ explicitly, that is for $\lambda_i^{(0)}$ and $x_i^{(0)}$ such that

$$\mathcal{A}_0 x_i^{(0)} = \lambda_i^{(0)} x_i^{(0)}.$$

Verify your answers.

$$A_0 = \begin{pmatrix} -2 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -2 \end{pmatrix}, \quad A_0 - \lambda I = \begin{pmatrix} -2-\lambda & 1 & 0 \\ 1 & -2-\lambda & 1 \\ 0 & 1 & -2-\lambda \end{pmatrix}, \quad \det(A_0 - \lambda I) = (-2-\lambda)\left[(-2-\lambda)^2 - 1\right] + 2 + \lambda$$

$$\det(A_0 - \lambda I) = 0, \quad (-2-\lambda)\left[(-2-\lambda)^2 - 1\right] + 2 + \lambda = 0, \quad (-2-\lambda)\left((-2-\lambda)^2 - 1 - 1\right) = 0$$

$$(\lambda+2)\left((-2-\lambda)^2 - 2\right) = 0, \quad (-2-\lambda)^2 - 2 = 0 \quad \therefore \quad -\lambda - 2 = \pm\sqrt{2} \quad \therefore \quad \lambda = \mp\sqrt{2} - 2, \quad \lambda = -2$$

$$A_0 x_i^{(0)} = \lambda_i^{(0)} x_i^{(0)} : \quad \begin{pmatrix} -2 & 1 & 0 \\ 1 & -2 & 1 \\ 0 & 1 & -2 \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} = \lambda_i^{(0)} \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix}, \quad \begin{aligned} -2\alpha + \beta &= \lambda_i^{(0)}(\alpha) && (*) \\ \alpha - 2\beta + \gamma &= \lambda_i^{(0)}(\beta) && (**) \\ \beta - 2\gamma &= \lambda_i^{(0)}(\gamma) && (***) \end{aligned}$$

Equations $(*)$, $(**)$, $(***)$ imply $\alpha = \gamma$ or $-\alpha = \gamma$: $\beta = \pm\sqrt{2}$ or $\beta = 0$

$$\lambda_1^{(0)} = -\sqrt{2} - 2, \quad x_1^{(0)} = \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}, \quad \sqrt{1+2+1} = 2 \quad \therefore \quad x_1^{(0)} = \frac{1}{2}\begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}$$

$$\lambda_2^{(0)} = -2, \quad x_2^{(0)} = \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}, \quad \sqrt{1+1} = \sqrt{2} \quad \therefore \quad x_2^{(0)} = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}$$

$$\lambda_3^{(0)} = \sqrt{2} - 2 \quad x_3^{(0)} = \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}, \quad \sqrt{1+2+1} = 2 \quad \therefore \quad x_3^{(0)} = \frac{1}{2}\begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}$$

$$\boxed{\lambda_1^{(0)} = -\sqrt{2} - 2, \; x_1^{(0)} = \frac{1}{2}\begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix} \; : \; \lambda_2^{(0)} = -2, \; x_2^{(0)} = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix} \; : \; \lambda_3^{(0)} = \sqrt{2} - 2, \; x_3^{(0)} = \frac{1}{2}\begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}}$$

Problem 1: Continued

(b) Using the results of (a), calculate the first order correction to the eigenvalues.

$$\lambda_1^{(1)} = \langle x_1^{(0)} | A_1 | x_1^{(0)} \rangle = \frac{1}{2}(1 \; -\sqrt{2} \; 1) \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \frac{1}{2} \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix} = \frac{1}{2} \quad \therefore \quad \lambda_1^{(1)} = -\sqrt{2} - 2 + \frac{\epsilon}{2}$$

$$\lambda_2^{(1)} = \langle x_2^{(0)} | A_1 | x_2^{(0)} \rangle = \frac{1}{\sqrt{2}}(-1 \; 0 \; 1) \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix} = -1 \quad \therefore \quad \lambda_2^{(1)} = -2 - \epsilon$$

$$\lambda_3^{(1)} = \langle x_3^{(0)} | A_1 | x_3^{(0)} \rangle = \frac{1}{2}(1 \; \sqrt{2} \; 1) \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \frac{1}{2} \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix} = \frac{1}{2} \quad \therefore \quad \lambda_3^{(1)} = \sqrt{2} - 2 + \frac{\epsilon}{2}$$

$$\boxed{\lambda_1^{(1)} = -\sqrt{2} - 2 + \frac{\epsilon}{2}, \; \lambda_2^{(1)} = -2 - \epsilon, \; \lambda_3^{(1)} = \sqrt{2} - 2 + \frac{\epsilon}{2}}$$

(c) Calculate the first order corrections to the eigenvectors.

$$x_n^{(1)} = \sum_{j \neq n} \frac{(x_j^{(0)}, A_1 x_n^{(0)})}{\lambda_n^{(0)} - \lambda_j^{(0)}} x_j^{(0)}, \quad x_1^{(1)} = \frac{(x_2^{(0)}, A_1 x_1^{(0)})}{\lambda_1^{(0)} - \lambda_2^{(0)}} x_2^{(0)} + \frac{(x_3^{(0)}, A_1 x_1^{(0)})}{\lambda_1^{(0)} - \lambda_3^{(0)}} x_3^{(0)}$$

$$x_2^{(1)} = \frac{(x_1^{(0)}, A_1 x_2^{(0)})}{\lambda_2^{(0)} - \lambda_1^{(0)}} x_1^{(0)} + \frac{(x_3^{(0)}, A_1 x_2^{(0)})}{\lambda_2^{(0)} - \lambda_3^{(0)}} x_3^{(0)}, \quad x_3^{(1)} = \frac{(x_1^{(0)}, A_1 x_3^{(0)})}{\lambda_3^{(0)} - \lambda_1^{(0)}} x_1^{(0)} + \frac{(x_2^{(0)}, A_1 x_3^{(0)})}{\lambda_3^{(0)} - \lambda_2^{(0)}} x_2^{(0)}$$

$$x_1^{(1)} = \cancelto{0}{\frac{\frac{1}{\sqrt{2}}(-1 \; 0 \; 1) \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \frac{1}{2} \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}}{-\sqrt{2} - 2 + 2}} x_2^{(0)} + \frac{\frac{1}{2}(1 \; \sqrt{2} \; 1) \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \frac{1}{2} \begin{pmatrix} 1 \\ -\sqrt{2} \\ 1 \end{pmatrix}}{-\sqrt{2} - 2 - \sqrt{2} + 2} x_3^{(0)} = -\frac{1}{4\sqrt{2}} x_3^{(0)}$$

$$x_2^{(1)} = \cancelto{0}{\frac{\frac{1}{2}(1 \; -\sqrt{2} \; 1) \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}}{-2 + \sqrt{2} + 2}} x_1^{(0)} + \cancelto{0}{\frac{\frac{1}{2}(1 \; \sqrt{2} \; 1) \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix}}{-2 - \sqrt{2} + 2}} x_3^{(0)} = 0$$

$$x_3^{(1)} = \frac{\frac{1}{2}(1 \; -\sqrt{2} \; 1) \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \frac{1}{2} \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}}{\sqrt{2} - 2 + \sqrt{2} + 2} x_1^{(0)} + \cancelto{0}{\frac{\frac{1}{2}(-1 \; 0 \; 1) \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ \sqrt{2} \\ 1 \end{pmatrix}}{\sqrt{2} - 2 + 2}} x_2^{(0)} = \frac{1}{4\sqrt{2}} x_1^{(0)}$$

$$\boxed{x_1^{(1)} = -\frac{1}{4\sqrt{2}} x_3^{(0)}, \; x_2^{(1)} = 0, \; x_3^{(1)} = \frac{1}{4\sqrt{2}} x_1^{(0)}}$$

Problem 1: Continued

(d) Calculate the second order corrections to the eigenvalues.

$$\lambda_n^{(2)} = \sum_{j\neq n} \frac{|(x_j^{(0)}, A_1 x_n^{(0)})|^2}{\lambda_n^{(0)} - \lambda_j^{(0)}} \quad , \quad \lambda_1^{(2)} = \frac{|(x_2^{(0)}, A_1 x_1^{(0)})|^2}{\lambda_1^{(0)} - \lambda_2^{(0)}} + \frac{|(x_3^{(0)}, A_1 x_1^{(0)})|^2}{\lambda_1^{(0)} - \lambda_3^{(0)}}$$

$$\lambda_2^{(2)} = \frac{|(x_1^{(0)}, A_1 x_2^{(0)})|^2}{\lambda_2^{(0)} - \lambda_1^{(0)}} + \frac{|(x_3^{(0)}, A_1 x_2^{(0)})|^2}{\lambda_2^{(0)} - \lambda_3^{(0)}} \quad , \quad \lambda_3^{(2)} = \frac{|(x_1^{(0)}, A_1 x_3^{(0)})|^2}{\lambda_3^{(0)} - \lambda_1^{(0)}} + \frac{|(x_2^{(0)}, A_1 x_3^{(0)})|^2}{\lambda_3^{(0)} - \lambda_2^{(0)}}$$

$$\lambda_1^{(2)} = \cancelto{0}{\frac{\left|\frac{1}{\sqrt{2}}\begin{pmatrix}-1 & 0 & 1\end{pmatrix}\begin{pmatrix}0&0&1\\0&0&0\\1&0&0\end{pmatrix}\frac{1}{2}\begin{pmatrix}1\\-\sqrt{2}\\1\end{pmatrix}\right|^2}{-\sqrt{2}-2+2}} + \frac{\left|\frac{1}{2}\begin{pmatrix}1 & \sqrt{2} & 1\end{pmatrix}\begin{pmatrix}0&0&1\\0&0&0\\1&0&0\end{pmatrix}\frac{1}{2}\begin{pmatrix}1\\-\sqrt{2}\\1\end{pmatrix}\right|^2}{-\sqrt{2}-2-\sqrt{2}+2} = -\frac{1}{8\sqrt{2}}\epsilon^2$$

$$\lambda_2^{(2)} = \cancelto{0}{\frac{\left|\frac{1}{2}\begin{pmatrix}1 & -\sqrt{2} & 1\end{pmatrix}\begin{pmatrix}0&0&1\\0&0&0\\1&0&0\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}-1\\0\\1\end{pmatrix}\right|^2}{-2+\sqrt{2}+2}} + \cancelto{0}{\frac{\left|\frac{1}{2}\begin{pmatrix}1 & \sqrt{2} & 1\end{pmatrix}\begin{pmatrix}0&0&1\\0&0&0\\1&0&0\end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix}-1\\0\\1\end{pmatrix}\right|^2}{-2-\sqrt{2}+2}} = 0\,\epsilon^2$$

$$\lambda_3^{(2)} = \frac{\left|\frac{1}{2}\begin{pmatrix}1 & -\sqrt{2} & 1\end{pmatrix}\begin{pmatrix}0&0&1\\0&0&0\\1&0&0\end{pmatrix}\frac{1}{2}\begin{pmatrix}1\\\sqrt{2}\\1\end{pmatrix}\right|^2}{\sqrt{2}-2+\sqrt{2}+2} + \cancelto{0}{\frac{\left|\frac{1}{\sqrt{2}}\begin{pmatrix}-1 & 0 & 1\end{pmatrix}\begin{pmatrix}0&0&1\\0&0&0\\1&0&0\end{pmatrix}\frac{1}{2}\begin{pmatrix}1\\\sqrt{2}\\1\end{pmatrix}\right|^2}{\sqrt{2}-2+2}} = \frac{1}{8\sqrt{2}}\epsilon^2$$

$$\boxed{\lambda_1^{(2)} = -\sqrt{2} - 2 + \frac{\epsilon}{2} - \frac{\epsilon^2}{8\sqrt{2}} \; , \; \lambda_2^{(2)} = -2 - \epsilon \; , \; \lambda_3^{(2)} = \sqrt{2} - 2 + \frac{\epsilon}{2} + \frac{\epsilon^2}{8\sqrt{2}}}$$

Problem 1: Review

Procedure:

- Calculate the eigenvalues and eigenvectors of the $\mathcal{A}_0$ matrix.
- Find the first order correction to the eigenvalues with

$$\lambda_i^{(1)} = \langle x_i^{(0)} | \mathcal{A}_1 | x_i^{(0)} \rangle \, .$$

- Find the first order correction to the eigenvectors with

$$x_n^{(1)} = \sum_{j \neq n} \frac{\langle x_j^{(0)} | \mathcal{A}_1 | x_n^{(0)} \rangle}{\lambda_n^{(0)} - \lambda_j^{(0)}} x_j^{(0)}.$$

- Find the second order correction to the eigenvalues with

$$\lambda_n^{(2)} = \sum_{j \neq n} \frac{| \langle x_j^{(0)} | \mathcal{A}_1 | x_n^{(0)} \rangle |^2}{\lambda_n^{(0)} - \lambda_j^{(0)}}.$$

Key Concepts:

- We use predefined formulas to find the corrections to eigenvalues and eigenvectors.

Variations:

- We can be given a different matrix for $\mathcal{A}_0$ and $\mathcal{A}_1$.
  - This would give us different end results but with the same procedure.

Problem 2:

Repeat the above problem (Problem 1) using MATHEMATICA or any other software.

PHYS 5013 HW 9

Problem 2:

Part a.)

In[•]:=
```
A0 = {{-2, 1, 0}, {1, -2, 1}, {0, 1, -2}};
A1 = {{0, 0, 1}, {0, 0, 0}, {1, 0, 0}};
Eigenvalues[A0]
```

Out[•]= $\{-2-\sqrt{2},\ -2,\ -2+\sqrt{2}\}$

In[•]:=
```
Eigenvectors[A0]
```

Out[•]= $\{\{1,\ -\sqrt{2},\ 1\},\ \{-1,\ 0,\ 1\},\ \{1,\ \sqrt{2},\ 1\}\}$

In[•]:=
```
a1 = Normalize[{1, -Sqrt[2], 1}];
```

In[•]:=
```
a2 = Normalize[{-1, 0, 1}];
```

In[•]:=
```
a3 = Normalize[{1, Sqrt[2], 1}];
e1 = -2 - Sqrt[2];
e2 = -2;
e3 = -2 + Sqrt[2];
```

Part b.)

In[•]:=
```
Transpose[a1].A1.a1
```

Out[•]= $\frac{1}{2}$

Therefore the first order correction to our first eigenvalue is:

In[•]:= $-2-\sqrt{2}+\frac{\varepsilon}{2};$

```
Transpose[a2].A1.a2
```

Out[•]= -1

Therefore the first order correction to our second eigenvalue is:

In[•]:= $-2-\varepsilon;$

```
Transpose[a3].A1.a3
```

Out[•]= $\frac{1}{2}$

Therefore the first order correction to our third eigenvalue is:

$$-2+\sqrt{2}+\frac{\varepsilon}{2};$$

Part c.)

First order correction for the first eigenvector is:

In[∘]:= (Transpose[a2].A1.a1) / (e1 - e2) * a2 + (Transpose[a3].A1.a1) / (e1 - e3) * a3

Out[∘]= $\left\{-\frac{1}{8\sqrt{2}}, -\frac{1}{8}, -\frac{1}{8\sqrt{2}}\right\}$

First order correction for the second eigenvector is:

In[∘]:= (Transpose[a1].A1.a2) / (e2 - e1) * a1 + (Transpose[a3].A1.a2) / (e2 - e3) * a3

Out[∘]= {0, 0, 0}

First order correction for the third eigenvector is:

In[∘]:= (Transpose[a1].A1.a3) / (e3 - e1) * a1 + (Transpose[a2].A1.a3) / (e3 - e2) * a2

Out[∘]= $\left\{\frac{1}{8\sqrt{2}}, -\frac{1}{8}, \frac{1}{8\sqrt{2}}\right\}$

Part d.)

Second order correction for the first eigenvalue is:

In[∘]:= $(\text{Transpose[a2].A1.a1})^2 / (\text{e1} - \text{e2}) + (\text{Transpose[a3].A1.a1})^2 / (\text{e1} - \text{e3})$

Out[∘]= $-\frac{1}{8\sqrt{2}}$

Second order correction for the second eigenvalue is:

In[∘]:= $(\text{Transpose[a1].A1.a2})^2 / (\text{e2} - \text{e1}) + (\text{Transpose[a3].A1.a2})^2 / (\text{e2} - \text{e3})$

Out[∘]= 0

Second order correction for the third eigenvalue is:

In[∘]:= $(\text{Transpose[a1].A1.a3})^2 / (\text{e3} - \text{e1}) + (\text{Transpose[a2].A1.a3})^2 / (\text{e3} - \text{e2})$

Out[∘]= $\frac{1}{8\sqrt{2}}$

Therefore the second order correction for the first eigenvalue is:

$$-2-\sqrt{2}+\frac{\varepsilon}{2}-\frac{\varepsilon^2}{8\sqrt{2}};$$

Therefore the second order correction for the second eigenvalue is:

$-2-\varepsilon;$

Therefore the second order correction for the third eigenvalue is:

$$-2+\sqrt{2}+\frac{\varepsilon}{2}+\frac{\varepsilon^2}{8\sqrt{2}};$$

Problem 2: Review

Procedure:

- Transcribe the math in Problem 1 to MATHEMATICA code to show the same results.

Key Concepts:

- We can use ***Eigenvalues*** and ***Eigenvectors*** to find the eigenvalues and eigenvectors of a matrix in MATHEMATICA.
- We can use other common MATHEMATICA commands to execute the same procedure.

Variations:

- Since this problem is based off of Problem 1, the only way this problem can change is if Problem 1 changes.
- We could be asked to plot something.
  - We then would use the correct respective commands to plot what is being asked of us.

Problem 3:

You might question the wisdom of using perturbation theory in the days of computers, when we can solve many problems quickly. In this problem you may use MATHEMATICA to either do perturbation theory or solve the problem exactly.

Extend the above problem so $\mathcal{A}_0$ is a 20×20 matrix, and $\mathcal{A}_1$ is a 20×20 matrix with 1 in the far upper right and lower left corners. Determine the numerical value of the eigenvalue with the smallest magnitude in the unperturbed problem, and the numerical coefficient of the first and second order correction to the lowest eigenvalue. That is, find the best polynomial to second order in ϵ that fits the lowest eigenvalue.

When you calculate the eigenvectors of $\mathcal{A}_0$, be sure that they are normalized. The eigenvalues and eigenvectors will all be real, so you don't have to worry about complex conjugation.

Problem 3:

In[3]:=
```
ClearAll["Global'*"]
A0 = Table[Table[
    If[j == i, -2, 0] + If[j == i + 1, 1, 0] + If[j == i - 1, 1, 0], {i, 1, 20}], {j, 1, 20}];
A1 = Table[Table[If[i == 20 j, 1, 0] + If[20 i == j, 1, 0], {i, 1, 20}], {j, 1, 20}];
eigenValues = Eigenvalues[A0];
eigenVectors = Eigenvectors[A0];
normalizedEigenVectors = Table[Normalize[eigenVectors[[i]]], {i, 1, 20}];
min = N[Min[Abs[eigenValues]]]
```

Out[9]= 0.0223383

The smallest magnitude of the eigenvalues of A0 is above.

In[12]:=
```
position = Position[N[Abs[eigenValues]], min];
```

In[27]:=
```
location = position[[1]][[1]];
eigenOne =
 N[Dot[normalizedEigenVectors[[location]], A1, normalizedEigenVectors[[location]]]]
```

Out[28]= 0.00423116

So the first order correction is,

$0.022338347549742954 + 0.004231161353700883\,\varepsilon;$

In[30]:=

$$\text{eigenTwo} = \text{Total}\left[\text{Table}\left[\text{If}\left[j \neq \text{location}, \frac{\text{Dot[normalizedEigenVectors[[j]], A1, normalizedEigenVectors[[location]]]}^2}{\text{min} - \text{eigenValues[[j]]}}, 0\right], \{j, 1, 20\}\right]\right]$$

Out[30]= 0.00329638

So the second order correction is,

$0.022338347549742954 + 0.004231161353700883\,\varepsilon + 0.003296382242657708\,\varepsilon^2;$

Problem 3: Review

Procedure:

- Use the ***Table*** command recursively to define the matrices that we are asked for in the problem statement.
- Find the eigenvalues and eigenvectors of this new matrix, normalize them, and then use the ***N***, ***Min***, and ***Abs*** commands to find the smallest eigenvalue.
- Proceed to use the rest of the MATHEMATICA code to find the corrections to the eigenvalues that are asked of us.

Key Concepts:

- We can use predefined MATHEMATICA commands to find corrections to eigenvalues.
- Using the ***Table*** command allows us to easily define new matrices.

Variations:

- We could be asked to create different matrices.
  - This would change how we define our initial matrices, but not the overall procedure.

Problem 4:

Degenerate Perturbation Theory: Consider the matrix

$$\mathcal{A} = \mathcal{A}_0 + \epsilon \mathcal{A}_1$$

where

$$\mathcal{A}_0 = \begin{pmatrix} -2 & 1 & 1 \\ 1 & -2 & 1 \\ 1 & 1 & -2 \end{pmatrix}$$

and

$$\mathcal{A}_1 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}.$$

The matrix $\mathcal{A}$ has eigenvalues λ_i with eigenvectors x_i, so that

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

(a) Solve for the eigenvalues and normalized eigenvectors of $\mathcal{A}_0$ explicitly, that is for $\lambda_i^{(0)}$ and $x_i^{(0)}$ such that

$$\mathcal{A}_0 x_i^{(0)} = \lambda_i^{(0)} x_i^{(0)}.$$

Verify your answers.

$$A_0 - \lambda I = \begin{pmatrix} -2 & 1 & 1 \\ 1 & -2 & 1 \\ 1 & 1 & -2 \end{pmatrix} - \begin{pmatrix} \lambda & 0 & 0 \\ 0 & \lambda & 0 \\ 0 & 0 & \lambda \end{pmatrix} = \begin{pmatrix} -2-\lambda & 1 & 1 \\ 1 & -2-\lambda & 1 \\ 1 & 1 & -2-\lambda \end{pmatrix}$$

$$\det(A_0 - \lambda I) = (-2-\lambda)((-2-\lambda)^2 - 1) + 1(1+2+\lambda) + 1(1+2+\lambda) = (-2-\lambda)^3 + 8 + 3\lambda$$

$$(-2-\lambda)^3 + 8 + 3\lambda = -\cancel{8} - 12\lambda - 6\lambda^2 - \lambda^3 + \cancel{8} + 3\lambda = -9\lambda - 6\lambda^2 - \lambda^3 = 0$$

$$9\lambda + 6\lambda^2 + \lambda^3 = 0 \;,\; \lambda = 0 \;:\; 9 + 6\lambda + \lambda^2 = 0 \quad (\lambda+3)^2 = 0 \;\therefore\; \lambda = -3, -3$$

$$\hat{A}\vec{x} = \lambda\vec{x} \;,\quad \begin{pmatrix} -2 & 1 & 1 \\ 1 & -2 & 1 \\ 1 & 1 & -2 \end{pmatrix}\begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} = \lambda \begin{pmatrix} \alpha \\ \beta \\ \gamma \end{pmatrix} , \quad \begin{aligned} -2\alpha + \beta + \gamma &= \lambda\alpha \\ \alpha - 2\beta + \gamma &= \lambda\beta \\ \alpha + \beta - 2\gamma &= \lambda\gamma \end{aligned}$$

$$\lambda = 0 , \quad \begin{aligned} -2\alpha + \beta + \gamma &= 0 \\ \alpha - 2\beta + \gamma &= 0 \\ \alpha + \beta - 2\gamma &= 0 \end{aligned}$$

$$\begin{aligned} -2\alpha + \beta + \gamma &= 0 \\ 2\alpha - 4\beta + 2\gamma &= 0 \end{aligned} \Rightarrow -3\beta + 3\gamma = 0 \Rightarrow -\beta + \gamma = 0 \;\therefore\; \gamma = \beta$$

$$\begin{aligned} \alpha - 2\beta + \gamma &= 0 \\ 2\alpha + 2\beta - 4\gamma &= 0 \end{aligned} \Rightarrow 3\alpha - 3\gamma = 0 \Rightarrow \alpha - \gamma = 0 \;\therefore\; \alpha = \gamma$$

$$\lambda_2^{(0)} = 0 \;,\; \vec{x}_{2,1}^{(0)} = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

$$\lambda = -3 , \quad \begin{aligned} \alpha + \beta + \gamma &= 0 \\ \alpha + \beta + \gamma &= 0 \\ \alpha + \beta + \gamma &= 0 \end{aligned} \Rightarrow \begin{aligned} \alpha &= -\beta - \gamma \\ \beta &= -\alpha - \gamma \\ \gamma &= -\alpha - \beta \end{aligned} \Rightarrow \alpha, \beta, \gamma = 0 \text{ while } \begin{aligned} \alpha = 0 ,&\; \beta = -\gamma \\ \beta = 0 ,&\; \alpha = -\gamma \\ \gamma = 0 ,&\; \alpha = -\beta \end{aligned}$$

Problem 4: Continued

$$\lambda_1^{(0)} = -3 \, , \; \vec{x}_{1,1}^{(0)} = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix} : \lambda_1^{(0)} = -3 \, , \; \vec{x}_{1,2}^{(0)} = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}$$

$$\boxed{\lambda_2^{(0)} = 0 \, , \; \vec{x}_{2,1}^{(0)} = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} : \lambda_1^{(0)} = -3 \, , \; \vec{x}_{1,1}^{(0)} = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix} : \lambda_1^{(0)} = -3 \, , \; \vec{x}_{1,2}^{(0)} = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}}$$

(b) Using the results of (a), calculate the first order correction to the eigenvalues.

$$a_{11} = (x_{1,1}^{(0)}, A_1 x_{1,1}^{(0)}) \, , \; a_{12} = (x_{1,1}^{(0)}, A_1 x_{1,2}^{(0)}) \, , \; a_{22} = (x_{1,2}^{(0)}, A_1 x_{1,2}^{(0)})$$

$$a_{11} = \frac{1}{\sqrt{2}}(-1\ 0\ 1)\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix} = -1 \; : \; a_{12} = \frac{1}{\sqrt{2}}(-1\ 0\ 1)\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix} = -\frac{1}{2}$$

$$a_{22} = \frac{1}{\sqrt{2}}(-1\ 1\ 0)\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix} = 0 \; : \; a = \begin{pmatrix} -1 & -1/2 \\ -1/2 & 0 \end{pmatrix} , \; a - \lambda I = \begin{pmatrix} -1-\lambda & -1/2 \\ -1/2 & -\lambda \end{pmatrix}$$

$$\det(a - \lambda I) = -\lambda(-1-\lambda) - 1/4 = 0 \, , \quad \lambda^2 + \lambda - 1/4 = 0 \quad \therefore \quad \lambda = \frac{1}{2}(\pm\sqrt{2} - 1)$$

$$\lambda_1^{(1)} = -3 + \frac{1}{2}(\pm\sqrt{2} - 1)\epsilon$$

$$\lambda_2^{(1)} = \langle x_{2,1}^{(0)} | A_1 | x_{2,1}^{(0)} \rangle = \frac{1}{\sqrt{3}}(1\ 1\ 1)\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}\frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \frac{2}{3} \quad \therefore \quad \lambda_2^{(1)} = \frac{2\epsilon}{3}$$

$$\boxed{\lambda_1^{(1)} = -3 + \frac{1}{2}(\pm\sqrt{2} - 1)\epsilon \, , \; \lambda_2^{(1)} = \frac{2\epsilon}{3}}$$

(c) Calculate the second order corrections to the eigenvalues.

$$\lambda_{n,i}^{(2)} = \sum_{m \neq n} \sum_{j=1}^{M_n} \frac{|(x_{m,j}^{(0)}, A_1 x_{n,i}^{(0)})|^2}{\lambda_n^{(0)} - \lambda_m^{(0)}} \, , \; \lambda_{1,1}^{(2)} = \sum_{m \neq 1} \sum_{j=1}^{1} \frac{|(x_{2,1}^{(0)}, A_1 x_{1,1}^{(0)})|^2}{\lambda_1^{(0)} - \lambda_2^{(0)}} \, , \; \lambda_{1,2}^{(2)} = \sum_{m \neq 1} \sum_{j=1}^{1} \frac{|(x_{2,1}^{(0)}, A_1 x_{1,2}^{(0)})|^2}{\lambda_1^{(0)} - \lambda_2^{(0)}}$$

$$\lambda_{1,1}^{(2)} = \sum_{m \neq 1} \sum_{j=1}^{1} \frac{|(x_{2,1}^{(0)}, A_1 x_{1,1}^{(0)})|^2}{\lambda_1^{(0)} - \lambda_2^{(0)}} = \frac{\left| \frac{1}{\sqrt{3}}(1\ 1\ 1)\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 0 \\ 1 \end{pmatrix} \right|^2}{-3 - 0} = 0 \, , \quad \therefore \quad \lambda_{1,1}^{(2)} = -3 + \frac{1}{2}(\pm\sqrt{2} - 1)\epsilon$$

$$\lambda_{1,2}^{(2)} = \sum_{m \neq 1} \sum_{j=1}^{1} \frac{|(x_{2,1}^{(0)}, A_1 x_{1,2}^{(0)})|^2}{\lambda_1^{(0)} - \lambda_2^{(0)}} = \frac{\left| \frac{1}{\sqrt{3}}(1\ 1\ 1)\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix} \right|^2}{-3 - 0} = -\frac{1}{18} \, , \quad \therefore \quad \lambda_{1,2}^{(2)} = -3 + \frac{1}{2}(\pm\sqrt{2} - 1)\epsilon - \frac{\epsilon^2}{18}$$

Problem 4: Continued

$$\lambda_n^{(2)} = \sum_{j\neq n} \frac{|(x_j^{(0)}, A_1 x_n^{(0)})|^2}{\lambda_n^{(0)} - \lambda_j^{(0)}}, \quad \lambda_2^{(2)} = \frac{|(x_{1,1}^{(0)}, A_1 x_{2,1}^{(0)})|^2}{0-(-3)} + \frac{|(x_{1,2}^{(0)}, A_1 x_{2,1}^{(0)})|^2}{0-(-3)}$$

$$\lambda_2 = \frac{1}{3}\left|\frac{1}{\sqrt{2}}(-1\ 0\ 1)\cancelto{0}{\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}}\frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}\right|^2 + \frac{1}{3}\left|\frac{1}{\sqrt{2}}(-1\ 1\ 0)\cancelto{1}{\begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}}\frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}\right|^2 = \frac{1}{18}$$

$$\therefore \lambda_{2,1}^{(2)} = \frac{2\epsilon}{3} + \frac{\epsilon^2}{18}$$

$$\boxed{\lambda_{1,1}^{(2)} = -3 + \frac{1}{2}(\pm\sqrt{2}-1)\epsilon, \quad \lambda_{1,2}^{(2)} = -3 + \frac{1}{2}(\pm\sqrt{2}-1)\epsilon - \frac{\epsilon^2}{18}, \quad \lambda_{2,1}^{(2)} = \frac{2\epsilon}{3} + \frac{\epsilon^2}{18}}$$

Problem 4: Review

Procedure:

- Find the eigenvalues and eigenvectors of $\mathcal{A}_0$.
- To find the first order correction to the eigenvalues, find the eigenvalues of the matrix

$$a = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$$

  with

$$a_{11} = \langle x_{1,1}^{(0)} | \mathcal{A}_1 | x_{1,1}^{(0)} \rangle \quad a_{12} = a_{21} = \langle x_{1,1}^{(0)} | \mathcal{A}_1 | x_{1,2}^{(0)} \rangle \quad a_{22} = \langle x_{1,2}^{(0)} | \mathcal{A}_1 | x_{1,2}^{(0)} \rangle \, .$$

- Find the second order correction to the eigenvalues with

$$\lambda_{n,i}^{(2)} = \sum_{m \neq n} \sum_{j=1}^{\mu_n} \frac{| \langle x_{m,j}^{(0)} | \mathcal{A}_1 | x_{n,j}^{(0)} \rangle |^2}{\lambda_n^{(0)} - \lambda_m^{(0)}}$$

  where μ_n is the order of degeneracy for the eigenvalues.

Key Concepts:

- We use predefined formulas to find the corrections to eigenvalues and eigenvectors.

Variations:

- We can be given a different matrix for $\mathcal{A}_0$ and $\mathcal{A}_1$.
  - This would give us different end results but with the same procedure.