Homework Assignment #9 Math Methods

Due: Monday, November 15th, midnight

Instructions:

Reading Quiz #6 on the last part of chapter 5 was supposed to be due last Wednesday - but I never opened it up! So I have made it due for Wednesday of this week.

Reading Quiz #7 on chapter 5 is due on Wednesday of next week.

Below is the a list of questions and problems. It is not sufficient to simply obtain the correct answer. You must also explain your calculation, and each step so that it is clear that you understand the material.

Homework should be written legibly, on standard size paper. Do not write your homework up on scrap paper. If your work is illegible, it will be given a zero.

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 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

$$A_0 x_i^{(0)} = \lambda_i^{(0)} x_i^{(0)}$$

Verify your answers.

- (b) Using the results of (a), calculate the first order correction to the eigenvalues.
- (c) Calculate the first order corrections to the eigenvectors.
- (d) Calculate the second order corrections to the eigenvalues.

Please do all of the above by hand, and not using MATHEMATICA or any other software.

2. Repeat the above problem using MATHEMATICA or any other software.

- 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 tridiagonal 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.

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 A has eigenvalues λ_i with eigenvectors x_i , so that

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

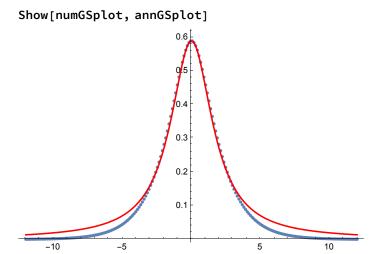
(a) Solve for the eigenvalues and normalized eigenvectors of \mathcal{A}_0 explicitly, that is for $\lambda_i^{(0)}$ and $x_i^{(0)}$ such that

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

Verify your answers.

- (b) Using the results of (a), calculate the first order correction to the eigenvalues.
- (c) Calculate the second order corrections to the eigenvalues.

Note that you are not asked to explicitly calculate the first order corrections to the eigenvectors.



Problem 3

The answer to this problem is identical to the one below, save that I have asked you to do it by hand here. I could scan my handwritten solutions, but simply referring you to the next section might be easier for you to read.

So, why did I make you write it out by hand? Because you need to know how to do this calculation, and one way to drill it is to actually do it out once by hand.

Problem 4

A0 = {{-2, 1, 0}, {1, -2, 1}, {0, 1, -2}};
A1 = {{0, 0, 1}, {0, 0, 0}, {1, 0, 0}};
MatrixForm[A0]

$$\begin{pmatrix}
-2 & 1 & 0 \\
1 & -2 & 1 \\
0 & 1 & -2
\end{pmatrix}$$

MatrixForm[A1]

$$\left(\begin{array}{cccc}
0 & 0 & 1 \\
0 & 0 & 0 \\
1 & 0 & 0
\end{array}\right)$$

(a) Solve unperturbed problem:

```
eout = Eigensystem[A0];
evals = {eval1, eval2, eval3} = eout[[1]]
temp = eout[[2]];
evecs = {evec1, evec2, evec3} = Table \left[\frac{\mathsf{temp}[[i]]}{\sqrt{\mathsf{temp}[[i]].\mathsf{temp}[[i]]}}, \{i, 1, 3\}\right];
\left\{-2-\sqrt{2}, -2, -2+\sqrt{2}\right\}
Check orthonormality:
Table[evecs[[i]].evecs[[j]], {i, 1, 3}, {j, 1, 3}] // MatrixForm
 0 1 0
 0 0 1
Verify our solutions:
MatrixForm[Simplify[A0.evec1 - eval1 evec1]]
MatrixForm[Simplify[A0.evec2 - eval2 evec2]]
MatrixForm[Simplify[A0.evec3 - eval3 evec3]]
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(b) First order corrections to eigenvalues:

```
\lambda_{1,(1)} = evec1.(A1.evec1)
\lambda_{2,(1)} = \text{evec2.}(A1.\text{evec2})
\lambda_{3,(1)} = evec3.(A1.evec3)
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(c) First order corrections to eigenvectors

$$\begin{aligned} x_{1,\,(1)} &= \frac{(\text{evec2.}(\text{A1.evec1}))}{\text{eval1-eval2}} \text{ evec2} + \frac{(\text{evec3.}(\text{A1.evec1}))}{\text{eval1-eval3}} \text{ evec3} \\ &\left\{ -\frac{1}{8\sqrt{2}}, -\frac{1}{8}, -\frac{1}{8\sqrt{2}} \right\} \\ x_{2,\,(1)} &= \frac{(\text{evec1.}(\text{A1.evec2}))}{\text{eval2-eval1}} \text{ evec1} + \frac{(\text{evec3.}(\text{A1.evec2}))}{\text{eval2-eval3}} \text{ evec3} \\ &\left\{ 0,\,0,\,0 \right\} \\ x_{3,\,(1)} &= \frac{(\text{evec1.}(\text{A1.evec3}))}{\text{eval3-eval1}} \text{ evec1} + \frac{(\text{evec2.}(\text{A1.evec3}))}{\text{eval3-eval2}} \text{ evec2} \\ &\left\{ \frac{1}{8\sqrt{2}}, -\frac{1}{8}, \frac{1}{8\sqrt{2}} \right\} \end{aligned}$$

(d) Second order correction to the eigenvalues

$$\lambda_{1,(2)} = \text{evec1.} \left(\text{A1.} x_{1,(1)} \right)$$

$$-\frac{1}{8\sqrt{2}}$$
 $\lambda_{2,(2)} = \text{evec2.} \left(\text{A1.} x_{2,(1)} \right)$
0
$$\lambda_{3,(2)} = \text{evec3.} \left(\text{A1.} x_{3,(1)} \right)$$

$$\frac{1}{8\sqrt{2}}$$

Check

echeck = Eigensystem[A0 +
$$\epsilon$$
 A1]
$$\left\{ \left\{ -2 - \epsilon, \frac{1}{2} \left(-4 + \epsilon - \sqrt{8 + \epsilon^2} \right), \frac{1}{2} \left(-4 + \epsilon + \sqrt{8 + \epsilon^2} \right) \right\}, \left\{ \left\{ -1, 0, 1 \right\}, \left\{ 1, -\frac{4 - \epsilon^2 - \epsilon \sqrt{8 + \epsilon^2}}{-3 \epsilon + \sqrt{8 + \epsilon^2}}, 1 \right\}, \left\{ 1, -\frac{-4 + \epsilon^2 - \epsilon \sqrt{8 + \epsilon^2}}{3 \epsilon + \sqrt{8 + \epsilon^2}}, 1 \right\} \right\} \right\}$$

Series[echeck[[1]],
$$\{\epsilon, 0, 2\}$$
]

$$\left\{-2-\varepsilon+0\,[\,\varepsilon\,]^{\,3}\,,\,\,\left(-2-\sqrt{2}\,\right)+\frac{\varepsilon}{2}-\frac{\varepsilon^{\,2}}{8\,\sqrt{2}}+0\,[\,\varepsilon\,]^{\,3}\,,\,\,\left(-2+\sqrt{2}\,\right)+\frac{\varepsilon}{2}+\frac{\varepsilon^{\,2}}{8\,\sqrt{2}}+0\,[\,\varepsilon\,]^{\,3}\right\}$$

```
TableForm[Series[echeck[[2]], \{\epsilon, 0, 1\}]]
- 1
           -\sqrt{2}-\frac{\epsilon}{2}+0[\epsilon]^2
1
           \sqrt{2} - \frac{\epsilon}{2} + 0 [\epsilon]^2
1
```

Problem 5

```
m0 = Table[If[i =: j, -2., If[Abs[i - j] =: 1, 1, 0]], {i, 1, 20}, {j, 1, 20}];
m1 = Table[0, {i, 1, 20}, {j, 1, 20}];
m1[[20, 1]] = 1;
m1[[1, 20]] = 1;
MatrixForm[m0 + ∈ m1]
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eout = Eigensystem[m0];
evals = eout[[1]];
evecs = Table \left[ \text{temp}[[j]] / \left( \sqrt{(\text{temp}[[j]].\text{temp}[[j]])} \right), \{j, 1, 20\} \right];
e0 = Min[evals]
-3.97766
```

```
temp = eout[[2]];
This is the lowest eigenvalue. Where is it in our list of eigenvalues?
Position[evals, e0]
\{ \{ 1 \} \}
```

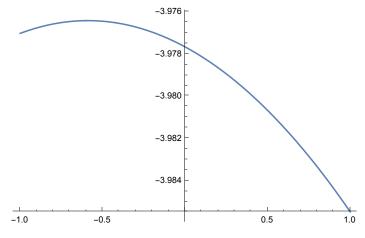
Aha! It is the very first one. This makes things easy. First order correction:

The second order correction involves a sum over states excluding the state we are perturbing. That's easy since we just exclude "j=1" from our sum.

Here's the series for the perturbation result for the lowest eigenvalue, and a plot of it:

e0fxn = e0 +
$$\epsilon$$
 e0₍₁₎ + ϵ ² e0₍₂₎
-3.97766 - 0.00423116 ϵ - 0.0035862 ϵ ²

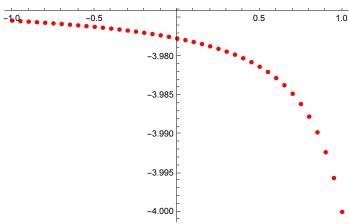
pertPlot = Plot[e0fxn, $\{\epsilon, -1, 1\}$]



Just for fun (not required) here is a plot of the exact eigenvalue as a function of ϵ .

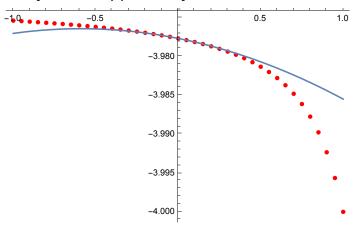
exact =

Table [temp = $m0 + \epsilon m1$; temp = Min[Eigenvalues[temp]]; { ϵ , temp}, { ϵ , -1, 1, .05}]; exactPlot = ListPlot[exact, PlotStyle → Red]



Comparing the two:

Show[exactPlot, pertPlot]



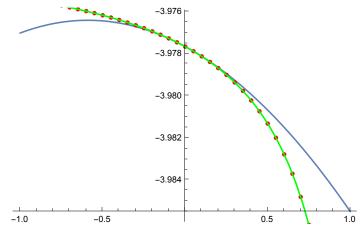
This is a good fit! To prove that to you, let's fit the data to a 12th order polynomial:

fitFxn = Fit[exact, Table
$$[\epsilon^n, \{n, 0, 12\}], \epsilon$$
]

- -3.97766-0.00423121 ϵ -0.00359174 ϵ^2 -0.00301073 ϵ^3 -0.0024152 ϵ^4 - $0.00196994 \in ^5$ - $0.00205212 \in ^6$ - $0.00179303 \in ^7$ - $0.000268952 \in ^8$ +
- $\textbf{0.000315875} \in ^9 \textbf{0.0011274} \in ^{10} \textbf{0.00162267} \in ^{11} \textbf{0.000571369} \in ^{12}$

We see that the first three terms in the series match our expansion very, very well! If we plot them all together we see:

fitPlot = Plot[fitFxn,
$$\{\varepsilon, -1, 1\}$$
, PlotStyle \rightarrow Green]; Show[pertPlot, exactPlot, fitPlot]



Our perturbation expansion obtained the correct coefficients for the power series expansion of the lowest eigenvalue. To obtain that from curve-fitting required fitting a 12th order polynomial to a large data set.

rect of
$$A_0$$
. The $\lambda_1 = 0$ $X_1^{(a)} = \frac{1}{\sqrt{3}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}$
 $\lambda_2 = -3 \begin{pmatrix} 1 \\ 1 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \begin{pmatrix} 2 \\ 1 \end{pmatrix} \begin{pmatrix}$

On particular is:

$$A_1 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

On fine exercise is:

$$A_1 = \begin{pmatrix} \times & (0) & \times & (0) \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

$$A_1 = \begin{pmatrix} \times & (0) & \times & (0) \\ 1 & 0 & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \frac{1}{3} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} = \frac{2}{3}$$

$$X_1^{(1)} = \begin{pmatrix} X_2^{(1)} & X_2^{(1)} & X_1^{(1)} & X_1^{(1)} & X_2^{(1)} & X_1^{(1)} & X_2^{(1)} & X_2^{($$

 $\times_{z_1}^{(3)} + \frac{-1}{9\sqrt{z}} \times_{z_1 z}^{(3)}$

The firm of the above answer depols upon our choice for
$$x_{21}$$
 of x_{212}^{1-3} - various thought as a reflect out $x_{1}^{(1)}$ explicitly as a closest of a reduct the the assumer is a depolat of our close of $x_{211}^{(1)}$.

$$x_{1}^{(1)} = \frac{1}{3\sqrt{6}} \left(\frac{1}{\sqrt{2}} \left(\frac{1}{-1} \right) - \frac{1}{3\sqrt{5}} \left(\frac{1}{-2} \right) \right)$$

$$= \frac{1}{18\sqrt{5}} \left(\frac{2}{-9} \right) = \frac{1}{18\sqrt{5}} \left(\frac{1}{-2} \right)$$

$$= \frac{1}{27} \left(\frac{2}{1} \right) - \frac{1}{3\sqrt{5}} \left(\frac{1}{-2} \right)$$

$$= \frac{1}{27} \left(\frac{2}{1} \right) - \frac{1}{3\sqrt{5}} \left(\frac{1}{-2} \right)$$

$$= \frac{1}{27} \left(\frac{2}{1} \right) - \frac{1}{3\sqrt{5}} \left(\frac{1}{-2} \right)$$

 $\lambda = \left[-\frac{2}{3} \pm \sqrt{\frac{4}{9} - 4(\frac{1}{3})} \right] / 2$

$$\lambda^{2} - \frac{1}{3} = \sqrt{\frac{1}{4}} + \frac{1}{3} = -\frac{1}{3} = \sqrt{\frac{4}{9}}$$

$$= -\frac{1}{3} \pm \frac{2}{3}$$

$$\begin{vmatrix} 1 & -\frac{1}{13} \\ -\frac{1}{13} & \frac{1}{13} \end{vmatrix} = -\frac{1}{3} \pm \sqrt{\frac{4}{9}}$$

$$+ \alpha - \frac{1}{13} = \frac{1}{3} = \frac{$$

$$\frac{1}{2\sqrt{6}} \left[\begin{array}{c} 3 \left(\frac{1}{1} \right) - \left(\frac{1}{1} \right) \\ \frac{1}{2\sqrt{6}} \left[\begin{array}{c} 2 \\ -4 \\ 2 \end{array} \right] = \frac{1}{\sqrt{6}} \left(\frac{1}{2} \right) \\ \frac{1}{2\sqrt{6}} \left[\begin{array}{c} 2 \\ -4 \\ 2 \end{array} \right] = \frac{1}{\sqrt{6}} \left(\frac{1}{2} \right) \\ \frac{1}{2\sqrt{6}} \left[\begin{array}{c} 2 \\ -4 \\ 2 \end{array} \right] = \frac{1}{\sqrt{6}} \left(\frac{1}{2} \right) \\ \frac{1}{2\sqrt{6}} \left[\begin{array}{c} 2 \\ -4 \\ 2 \end{array} \right] = \frac{1}{\sqrt{6}} \left(\frac{1}{2} \right) \left(\frac{1}{2} \right) \\ \frac{1}{2\sqrt{6}} \left(\frac{1}{2} \right) \\ \frac{1}{2\sqrt{6}} \left(\frac{1}{2} \right) \left(\frac{1}{2} \right) \\ \frac{1}{2\sqrt{6}} \left(\frac{1}{2$$

$$c_{22} \left(\begin{array}{c} x_{2}, 2 \\ x_{2}, 2 \end{array} \right), A_{1} q_{2,2}$$

$$-\frac{1}{\sqrt{6}} \stackrel{?}{q} \stackrel{?}{\sqrt{3}} \left(\begin{array}{c} 1 \\ 1 \\ -2 \end{array} \right) \left(\begin{array}{c} 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{array} \right) \left(\begin{array}{c} 1 \\ 1 \\ 1 \end{array} \right)$$

$$-\frac{1}{\sqrt{6}} \stackrel{?}{q} \stackrel{?}{\sqrt{3}} \left(\begin{array}{c} 1 \\ 1 \\ -2 \end{array} \right) \left(\begin{array}{c} 1 \\ 0 \\ 1 \end{array} \right) = -\frac{1}{27} \left(\begin{array}{c} 1 \\ 1 \\ -1 \end{array} \right) - \frac{1}{\sqrt{3}} \left(\begin{array}{c} -1\sqrt{3} \\ 1 \\ 1 \end{array} \right)$$

$$-\frac{1}{\sqrt{3}} \left(\begin{array}{c} -1\sqrt{3} \\ 1 \\ -1 \end{array} \right) - \frac{1}{\sqrt{3}} \left(\begin{array}{c} -1\sqrt{3} \\ 1 \\ 1 \end{array} \right)$$

$$= -\frac{1}{27} \left(\begin{array}{c} \sqrt{3} \\ -1 \end{array} \right) + \left(\begin{array}{c} -\sqrt{3} \\ 1 \\ 1 \end{array} \right)$$

$$= \frac{2}{27} \left(\begin{array}{c} 0 \\ 0 \end{array} \right)$$

$$= \frac{2}{27} \left(\begin{array}{c} 0 \\ 0 \end{array} \right)$$

$$= \frac{2}{27} \left(\begin{array}{c} 0 \\ 0 \end{array} \right)$$

$$= \frac{2}{27} \left(\begin{array}{c} 0 \\ 0 \end{array} \right)$$

$$= \frac{2}{27} \left(\begin{array}{c} 0 \\ 0 \end{array} \right)$$

$$= \frac{2}{27} \left(\begin{array}{c} 0 \\ 0 \end{array} \right)$$

Thus Ini 20 for both Jegunare againston-

Sommer
$$X_1 = \frac{1}{\sqrt{3}} \left(\begin{array}{c} 1 \\ 1 \end{array} \right) + \frac{2}{3} \left(\begin{array}{c} 1 \\ 1 \end{array} \right) + \frac{1}{3} \left(\begin{array}{c} 1 \\ 1 \end{array} \right)$$

$$\lambda_{2_1} \approx -3 - \epsilon + \phi \epsilon$$

$$3_{2_1} \approx \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix} + \phi \epsilon$$

$$\lambda_{2,2} \approx -3 + \frac{1}{3} \in -\frac{2}{27} \in^{2}$$

$$\frac{3}{2} = \frac{1}{\sqrt{6}} \left(\frac{1}{2} \right) + \left(-\sqrt{\frac{2}{3}} \right) = \left(\frac{1}{1} \right)$$