CHEM 5641 - PS1

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Problem 1. Consider 3-dimensional vectors $\mathbf{a}$ and $\mathbf{b}$ that are both in the basis $\{\vec{e}_i\}$, where $\vec{e}_i \cdot \vec{e}_j = \delta_{ij}$ (δ_{ij} is the Kronecker delta)

$$\mathbf{a} = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}, \quad \mathbf{b} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}$$

Compute $\mathbf{a}^\dagger \mathbf{b}$

Solution 1.

$$\begin{aligned} \mathbf{a}^\dagger \mathbf{b} &= \begin{pmatrix} 1 & 2 & 3 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \\ &= 1 \cdot 0 + 2 \cdot 1 + 3 \cdot 0 \\ &= 2 \end{aligned}$$

Problem 2. Given

$$\mathbf{a} = \begin{pmatrix} -i \\ 2i + 1 \\ 2 \end{pmatrix}$$

compute $\mathbf{a}^\dagger$

Solution 2.

$$\mathbf{a}^\dagger = \begin{pmatrix} i & 1 - 2i & 2 \end{pmatrix}$$

Problem 3. Given a square matrix

$$\mathbf{A} = \begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix},$$

(a) Compute the determinant of $\mathbf{A}$, $\det(\mathbf{A})$

(b) Compute the inverse of $\mathbf{A}$, $\mathbf{A}^{-1}$

(c) Find the eigenvalues of $\mathbf{A}$ and the eigenvectors corresponding to each eigenvalue

(d) Please normalize the eigenvectors, if they are not normalized in the previous question. Does the normalized eigenvector correspond to the same eigenvalue as the unnormalized one?

(e) Show that $\mathbf{A}$ is a Hermitian matrix

Solution 3.a.

$$\begin{aligned}
|\mathbf{A}| &= \begin{vmatrix} 1 & 1 \\ 1 & 2 \end{vmatrix} \\
&= 1 \cdot 2 - 1 \cdot 1 \\
&= 1
\end{aligned}$$

Solution 3.b.

$$\begin{aligned}
\mathbf{A}^{-1} &= \frac{1}{\det(\mathbf{A})} adj(\mathbf{A}) \\
&= \frac{1}{1 \cdot 2 - 1 \cdot 1} \begin{pmatrix} 2 & -1 \\ -1 & 1 \end{pmatrix} \\
\mathbf{A}^{-1} &= \begin{pmatrix} 2 & -1 \\ -1 & 1 \end{pmatrix}
\end{aligned}$$

Solution 3.c.

$$\begin{aligned}
|\mathbf{A} - \lambda \mathbf{I}| = 0 &= \begin{vmatrix} 1-\lambda & 1 \\ 1 & 2-\lambda \end{vmatrix} \\
&= (1-\lambda)(2-\lambda) - 1 \cdot 1 \\
&= \lambda^2 - 3\lambda + 1 \\
\rightarrow \quad \lambda &= \underline{\frac{3+\sqrt{5}}{2}, \frac{3-\sqrt{5}}{2}}
\end{aligned}$$

Plugging in the eigenvalues, we have

$$
\begin{aligned}
|\mathbf{A} - \lambda_1 \mathbf{I}|\mathbf{v}_1 = 0 &= \begin{vmatrix} \frac{-(1+\sqrt{5})}{2} & 1 \\ 1 & \frac{1-\sqrt{5}}{2} \end{vmatrix} \mathbf{v}_1 \\
\mathbf{v}_1 &= \underline{\begin{pmatrix} 2 \\ 1+\sqrt{5} \end{pmatrix}}
\end{aligned}
$$

$$
\begin{aligned}
|\mathbf{A} - \lambda_2 \mathbf{I}|\mathbf{v}_2 = 0 &= \begin{vmatrix} \frac{-1+\sqrt{5}}{2} & 1 \\ 1 & \frac{1+\sqrt{5}}{2} \end{vmatrix} \mathbf{v}_2 \\
\mathbf{v}_2 &= \underline{\begin{pmatrix} 2 \\ 1-\sqrt{5} \end{pmatrix}}
\end{aligned}
$$

Solution 3.d.

$$
\begin{aligned}
\hat{\mathbf{v}}_1 &= \frac{\mathbf{v}_1}{|\mathbf{v}_1|} \\
&= \frac{1}{\sqrt{4 + (1 + 2\sqrt{5} + 5)}} \mathbf{v}_1 \\
&= \frac{1}{\sqrt{10 + 2\sqrt{5}}} \mathbf{v}_1
\end{aligned}
$$

$$
\begin{aligned}
\hat{\mathbf{v}}_2 &= \frac{\mathbf{v}_2}{|\mathbf{v}_2|} \\
&= \frac{1}{\sqrt{4 + (1 - 2\sqrt{5} + 5)}} \mathbf{v}_2 \\
&= \frac{1}{\sqrt{10 - 2\sqrt{5}}} \mathbf{v}_2
\end{aligned}
$$

These do correspond to the same eigenvalues as the un-normalized ones because any scalar value multiplied by 0 has the same result.

Solution 3.e. In a Hermitian matrix, $\mathbf{A} = \mathbf{A}^\dagger$. Applying this, we see:

$$
\begin{aligned}
\mathbf{A} &= \begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix} \\
\mathbf{A}^\dagger = \left(\mathbf{A}^T\right)^* &= \begin{pmatrix} 1 & 1 \\ 1 & 2 \end{pmatrix}
\end{aligned}
$$

Both are the same so matrix $\mathbf{A}$ is Hermitian and its determinant is real.

Problem 4. Given a complete orthonormal basis $\{|i\rangle\}$, $i = 1, 2, \ldots, N$.
Let $|a\rangle = -i\,|1\rangle + 3.5\,|2\rangle$,
Let $|b\rangle = 0.1\,|1\rangle + i\,|2\rangle$.
Compute $\langle b|a\rangle$

Solution 4.

$$\begin{aligned} \langle b| &= 0.1\,\langle 1| - i\,\langle 2| \\ \rightarrow \qquad \langle b|a\rangle &= (-i \cdot 0.1)\,\langle 1|1\rangle + (-i \cdot 3.5)\,\langle 2|2\rangle \\ &= -3.6i \end{aligned}$$

Problem 5. Please login to Discovery, either through the terminal or through Open On Demand (OOD). Launch "Gaussian" if you are doing it through OOD; launch GaussView if you are doing it through the terminal. Build a hydrogen molecule in GaussView. Take a screenshot to show that you have successfully completed this task.

Solution 5. I don't have access to Gaussian so I ran an SSH from Windows into the cluster and did it with a few lines of Python in ASE.