Linear Algebra for Chemists — Assignment 8

by Yuval Bernard
ID. 211860754

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Question 1. Define the Fibonacci sequence as follows:

$$a_0 = 0, \quad a_1 = 1, \quad a_n = a_{n-1} + a_{n-2} \quad \text{for} \quad n > 1.$$

Let

$$A = \begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix} \quad \text{and} \quad \vec{v}_n = \begin{bmatrix} a_n \\ a_{n+1} \end{bmatrix}.$$

a) On one side,

$$\vec{v}_{n+1} = \begin{bmatrix} a_{n+1} \\ a_{n+2} \end{bmatrix},$$

and on the other side

$$A\,\vec{v}_n = \begin{bmatrix} 0 & 1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} a_n \\ a_{n+1} \end{bmatrix} = \begin{bmatrix} a_{n+1} \\ a_n + a_{n+1} \end{bmatrix}.$$

The the definition of the Fibonacci sequence, $a_n + a_{n+1} = a_{n+2}$, which verifies that

$$\vec{v}_{n+1} = A\,\vec{v}_n = \begin{bmatrix} a_{n+1} \\ a_{n+2} \end{bmatrix}.$$

b) To diagonalize A we find its eigenvalues and eigenvectors.

$$|A - \lambda I| = \begin{vmatrix} -\lambda & 1 \\ 1 & 1-\lambda \end{vmatrix} = 0$$

$$\lambda^2 - \lambda - 1 = 0.$$

$$\lambda_{1,2} = \frac{1 \pm \sqrt{1+4}}{2} = \frac{1 \pm \sqrt{5}}{2}.$$

$$A - \lambda_{1,2} I = \begin{bmatrix} -\frac{1\pm\sqrt{5}}{2} & 1 \\ 1 & 1 - \frac{1\pm\sqrt{5}}{2} \end{bmatrix} = \begin{bmatrix} -\frac{1\pm\sqrt{5}}{2} & 1 \\ 1 & \frac{1\mp\sqrt{5}}{2} \end{bmatrix} \sim \begin{bmatrix} -\frac{1\pm\sqrt{5}}{2} & 1 \\ 0 & \frac{1\mp\sqrt{5}}{2} + \frac{2}{1\pm\sqrt{5}} \end{bmatrix}.$$

The eigenvectors of A are

$$\vec{w}_{1,2} = \begin{bmatrix} 2 \\ 1 \pm \sqrt{5} \end{bmatrix}$$

Factorize A as

$$A = P\,D\,P^{-1}.$$

such that

$$P = \begin{bmatrix} 1 & 1 \\ \frac{1+\sqrt{5}}{2} & \frac{1-\sqrt{5}}{2} \end{bmatrix}, \quad D = \begin{bmatrix} \frac{1+\sqrt{5}}{2} & 0 \\ 0 & \frac{1-\sqrt{5}}{2} \end{bmatrix}.$$

Calculate P^{-1}. For a 2×2 matrix B,

$$B^{-1} = \frac{1}{b_{11}\,b_{22} - b_{12}\,b_{21}} \begin{bmatrix} b_{22} & -b_{12} \\ -b_{21} & b_{11} \end{bmatrix}.$$

$$P^{-1} = \frac{1}{\frac{1}{2}\times(-2\sqrt{5})} \begin{bmatrix} \frac{1-\sqrt{5}}{2} & -1 \\ -\frac{1+\sqrt{5}}{2} & 1 \end{bmatrix} = -\frac{1}{\sqrt{5}} \begin{bmatrix} \frac{1-\sqrt{5}}{2} & -1 \\ -\frac{1+\sqrt{5}}{2} & 1 \end{bmatrix} = \begin{bmatrix} -\frac{1-\sqrt{5}}{2\sqrt{5}} & \frac{1}{\sqrt{5}} \\ \frac{1+\sqrt{5}}{2\sqrt{5}} & -\frac{1}{\sqrt{5}} \end{bmatrix}$$

Use the formula

$$A^n = P D^n P^{-1}$$

to get an expression for A^n:

$$\begin{aligned}
A^n &= \begin{bmatrix} 1 & 1 \\ \frac{1+\sqrt{5}}{2} & \frac{1-\sqrt{5}}{2} \end{bmatrix} \begin{bmatrix} \left(\frac{1+\sqrt{5}}{2}\right)^n & 0 \\ 0 & \left(\frac{1-\sqrt{5}}{2}\right)^n \end{bmatrix} \begin{bmatrix} -\frac{1-\sqrt{5}}{2\sqrt{5}} & \frac{1}{\sqrt{5}} \\ \frac{1+\sqrt{5}}{2\sqrt{5}} & -\frac{1}{\sqrt{5}} \end{bmatrix} \\
&= \begin{bmatrix} 1 & 1 \\ \frac{1+\sqrt{5}}{2} & \frac{1-\sqrt{5}}{2} \end{bmatrix} \begin{bmatrix} -\left(\frac{1+\sqrt{5}}{2}\right)^n \left(\frac{1-\sqrt{5}}{2}\right) \frac{1}{\sqrt{5}} & \left(\frac{1+\sqrt{5}}{2}\right)^n \frac{1}{\sqrt{5}} \\ \left(\frac{1-\sqrt{5}}{2}\right)^n \left(\frac{1+\sqrt{5}}{2}\right) \frac{1}{\sqrt{5}} & -\left(\frac{1-\sqrt{5}}{2}\right)^n \frac{1}{\sqrt{5}} \end{bmatrix} \\
&= \frac{1}{\sqrt{5}} \begin{bmatrix} 1 & 1 \\ \frac{1+\sqrt{5}}{2} & \frac{1-\sqrt{5}}{2} \end{bmatrix} \begin{bmatrix} \left(\frac{1+\sqrt{5}}{2}\right)^{n-1} & \left(\frac{1+\sqrt{5}}{2}\right)^n \\ -\left(\frac{1-\sqrt{5}}{2}\right)^{n-1} & -\left(\frac{1-\sqrt{5}}{2}\right)^n \end{bmatrix} \\
&= \frac{1}{\sqrt{5}} \begin{bmatrix} \left(\frac{1+\sqrt{5}}{2}\right)^{n-1} - \left(\frac{1-\sqrt{5}}{2}\right)^{n-1} & \left(\frac{1+\sqrt{5}}{2}\right)^n - \left(\frac{1-\sqrt{5}}{2}\right)^n \\ \left(\frac{1+\sqrt{5}}{2}\right)^n - \left(\frac{1-\sqrt{5}}{2}\right)^n & \left(\frac{1+\sqrt{5}}{2}\right)^{n+1} - \left(\frac{1-\sqrt{5}}{2}\right)^{n+1} \end{bmatrix}.
\end{aligned}$$

c)

$$\begin{aligned}
\vec{v}_n = A^n\,\vec{v}_0 &= \frac{1}{\sqrt{5}} \begin{bmatrix} \left(\frac{1+\sqrt{5}}{2}\right)^{n-1} - \left(\frac{1-\sqrt{5}}{2}\right)^{n-1} & \left(\frac{1+\sqrt{5}}{2}\right)^n - \left(\frac{1-\sqrt{5}}{2}\right)^n \\ \left(\frac{1+\sqrt{5}}{2}\right)^n - \left(\frac{1-\sqrt{5}}{2}\right)^n & \left(\frac{1+\sqrt{5}}{2}\right)^{n+1} - \left(\frac{1-\sqrt{5}}{2}\right)^{n+1} \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \end{bmatrix} \\
&= \frac{1}{\sqrt{5}} \begin{bmatrix} \left(\frac{1+\sqrt{5}}{2}\right)^{n-1} - \left(\frac{1-\sqrt{5}}{2}\right)^{n-1} & \left(\frac{1+\sqrt{5}}{2}\right)^n - \left(\frac{1-\sqrt{5}}{2}\right)^n \\ \left(\frac{1+\sqrt{5}}{2}\right)^n - \left(\frac{1-\sqrt{5}}{2}\right)^n & \left(\frac{1+\sqrt{5}}{2}\right)^{n+1} - \left(\frac{1-\sqrt{5}}{2}\right)^{n+1} \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix} \\
&= \frac{1}{\sqrt{5}} \begin{bmatrix} \left(\frac{1+\sqrt{5}}{2}\right)^n - \left(\frac{1-\sqrt{5}}{2}\right)^n \\ \left(\frac{1+\sqrt{5}}{2}\right)^{n+1} - \left(\frac{1-\sqrt{5}}{2}\right)^{n+1} \end{bmatrix}.
\end{aligned}$$

Using the definition for $\vec{v}_n$, we conclude that

$$a_n = \left(\frac{1+\sqrt{5}}{2}\right)^n - \left(\frac{1-\sqrt{5}}{2}\right)^n.$$

Question 2. Perform eigendecomposition on the following:

a)

$$A = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 2 & 4 \\ 1 & -1 & 3 \end{bmatrix}.$$

Find eigenvalues.

$$\begin{aligned} |A - \lambda I| &= \begin{vmatrix} 1-\lambda & 0 & 0 \\ 1 & 2-\lambda & 4 \\ 1 & -1 & 3-\lambda \end{vmatrix} \\ &= (1-\lambda)\,[(2-\lambda)\,(3-\lambda)+4] \\ &= (1-\lambda)\,(\lambda^2 - 5\,\lambda + 10) = 0. \end{aligned}$$

$$\lambda_1 = 1, \quad \lambda_{2,3} = \frac{5 \pm \sqrt{5^2 - 40}}{2} = \frac{5 \pm \sqrt{15}\,\mathrm{i}}{2}.$$

Calculate eigenvectors. For $\lambda_1 = 1$,

$$A - \lambda_1 I = \begin{bmatrix} 0 & 0 & 0 \\ 1 & 1 & 4 \\ 1 & -1 & 2 \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 4 \\ 2 & 0 & 6 \\ 0 & 0 & 0 \end{bmatrix} \sim \begin{bmatrix} 1 & 1 & 4 \\ 1 & 0 & 3 \\ 0 & 0 & 0 \end{bmatrix} \sim \begin{bmatrix} 1 & 0 & 3 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \end{bmatrix}.$$

$$w_1 = \begin{bmatrix} 3 \\ 1 \\ -1 \end{bmatrix}.$$

For $\lambda_2 = \frac{5+\sqrt{15}\,\mathrm{i}}{2}$,

$$\begin{aligned} A - \lambda_2 I &= \begin{bmatrix} 1 - \frac{5+\sqrt{15}\,\mathrm{i}}{2} & 0 & 0 \\ 1 & 2 - \frac{5+\sqrt{15}\,\mathrm{i}}{2} & 4 \\ 1 & -1 & 3 - \frac{5+\sqrt{15}\,\mathrm{i}}{2} \end{bmatrix} \\ &= \begin{bmatrix} -\frac{3+\sqrt{15}\,\mathrm{i}}{2} & 0 & 0 \\ 1 & -\frac{1+\sqrt{15}\,\mathrm{i}}{2} & 4 \\ 1 & -1 & \frac{1-\sqrt{15}\,\mathrm{i}}{2} \end{bmatrix}. \\ &\sim \begin{bmatrix} -\frac{3+\sqrt{15}\,\mathrm{i}}{2} & 0 & 0 \\ -\frac{2}{1+\sqrt{15}\,\mathrm{i}} & 1 & -4 \times \frac{2}{1+\sqrt{15}\,\mathrm{i}} \\ 1 & -1 & \frac{1-\sqrt{15}\,\mathrm{i}}{2} \end{bmatrix} \\ &= \begin{bmatrix} -\frac{3+\sqrt{15}\,\mathrm{i}}{2} & 0 & 0 \\ -\frac{2}{1+\sqrt{15}\,\mathrm{i}} & 1 & \frac{-1+\sqrt{15}\,\mathrm{i}}{2} \\ 1 & -1 & \frac{1-\sqrt{15}\,\mathrm{i}}{2} \end{bmatrix} \end{aligned}$$

$$w_2 = \begin{bmatrix} 0 \\ \frac{1-\sqrt{15}\,\mathrm{i}}{2} \\ 1 \end{bmatrix}$$

and for $\lambda_3 = \overline{\left(\frac{1+\sqrt{15}\,\mathrm{i}}{2}\right)}$,

$$w_3 = \bar{w}_2 = \begin{bmatrix} 0 \\ \frac{1+\sqrt{15}\,\mathrm{i}}{2} \\ 1 \end{bmatrix}.$$

In conclusion, P, D are

$$P = \begin{bmatrix} 0 & 0 & 3 \\ \frac{1-\sqrt{15}\,\mathrm{i}}{2} & \frac{1+\sqrt{15}\,\mathrm{i}}{2} & 1 \\ 1 & 1 & -1 \end{bmatrix}, \quad D = \begin{bmatrix} \frac{5+\sqrt{15}\,\mathrm{i}}{2} & 0 & 0 \\ 0 & \frac{5-\sqrt{15}\,\mathrm{i}}{2} & 0 \\ 0 & 0 & 1 \end{bmatrix}$$

b)

$$A = \begin{bmatrix} 3 & 1 & 1 \\ 0 & 2 & 1 \\ 0 & 0 & 1 \end{bmatrix}.$$

The eigenvalues of a triangular matrix are on the diagonal: $\lambda_{1,2,3} = 3, 2, 1$. Find associated eigenvectors.

$$[A - \lambda_1 I] \;=\; \begin{bmatrix} 0 & 1 & 1 \\ 0 & -1 & 1 \\ 0 & 0 & -2 \end{bmatrix}.$$

$$w_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}.$$

$$[A - \lambda_2 I] = \begin{bmatrix} 1 & 1 & 1 \\ 0 & 0 & 1 \\ 0 & 0 & -1 \end{bmatrix}.$$

$$w_2 = \begin{bmatrix} 1 \\ -1 \\ 0 \end{bmatrix}.$$

$$[A - \lambda_3 I] = \begin{bmatrix} 2 & 1 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \end{bmatrix}.$$

$$w_3 = \begin{bmatrix} 0 \\ 1 \\ -1 \end{bmatrix}.$$

P, D are

$$P = \begin{bmatrix} 1 & 1 & 0 \\ 0 & -1 & 1 \\ 0 & 0 & -1 \end{bmatrix}, \quad D = \begin{bmatrix} 3 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{bmatrix}.$$

c)

$$A = \begin{bmatrix} 1 & 4 \\ 4 & 1 \end{bmatrix}.$$

$$|A - \lambda I| = \begin{vmatrix} 1-\lambda & 4 \\ 4 & 1-\lambda \end{vmatrix} = \lambda^2 - 2\lambda - 15 = 0$$

$$\lambda_{1,2} = \frac{2 \pm \sqrt{4+60}}{2} = 5, -3.$$

Find associated eigenvectors. For $\lambda_1 = 5$,

$$[A - \lambda_1 I] = \begin{bmatrix} -4 & 4 \\ 4 & -4 \end{bmatrix}.$$

$$w_1 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}.$$

For $\lambda_2 = -3$,

$$[A - \lambda_2 I] = \begin{bmatrix} 4 & 4 \\ 4 & 4 \end{bmatrix}.$$

$$w_2 = \begin{bmatrix} 1 \\ -1 \end{bmatrix}.$$

P, D are

$$P = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \quad D = \begin{bmatrix} 5 & 0 \\ 0 & -3 \end{bmatrix}.$$

d)

$$A = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 3 \\ 0 & 0 & 1 & 3 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

The eigenvalues of a triangular matrix are on the diagonal. $\lambda_{1,2,3,4} \equiv \lambda = 1$. Find eigenvectors.

$$[A - \lambda I] = \begin{bmatrix} 0 & 1 & 1 & 1 \\ 0 & 0 & 2 & 3 \\ 0 & 0 & 0 & 3 \\ 0 & 0 & 0 & 0 \end{bmatrix}.$$

The geometric multiplicity of the eigenvalue λ, that is, the dimension of the nullspace of $A - \lambda I$, is smaller than its algebraic multiplicity. A is therefore not diagonalizable.

e)

$$A = \begin{bmatrix} 3 & 2 \\ 0 & 5 \end{bmatrix}.$$

The matrix is triangular. $\lambda_{1,2} = 3, 5$. Find associated eigenvectors.

$$[A - \lambda_1 I] = \begin{bmatrix} 0 & 2 \\ 0 & 2 \end{bmatrix}.$$

$$w_1 = \begin{bmatrix} 1 \\ 0 \end{bmatrix}.$$

$$[A - \lambda_2 I] = \begin{bmatrix} -2 & 2 \\ 0 & 0 \end{bmatrix}.$$

$$w_2 = \begin{bmatrix} 1 \\ 1 \end{bmatrix}.$$

P, D are

$$P = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}, \quad D = \begin{bmatrix} 3 & 0 \\ 0 & 5 \end{bmatrix}.$$

Question 3. .

a) Show that if $P^{-1} A P = D$ then $A^n = P D^n P^{-1}$.

We shall use induction. For $n = 0$,

$$A^0 = I = P D^0 P^{-1} = P I P^{-1} = I.$$

For $n = 1$, start from

$$P^{-1} A P = D.$$

Multipliy by P on the left and by P^{-1} on the right to get

$$P P^{-1} A P P^{-1} = P D P^{-1}$$

$$A = P D P^{-1}.$$

Now assume that for $n = k$

$$A^k = P D^k P^{-1}.$$

For $n = k + 1$,

$$\begin{aligned} A^{k+1} = A^k A &= (P D^k P^{-1}) P D P^{-1} \\ &= P D^k P^{-1} P D P^{-1} \\ &= P D^k I D P^{-1} \\ &= P D^{k+1} P^{-1}. \end{aligned}$$

QED.

b) Given $A = \left[\begin{smallmatrix} 1 & 0 \\ 2 & 3 \end{smallmatrix}\right]$, calculate A^8. Diagonalize A.

A is triangular. The eigenvalues are $\lambda_{1,2}=1,3$. Find associated eigenvectors.

$$[A-\lambda_1 I]=\begin{bmatrix} 0 & 0 \\ 2 & 2 \end{bmatrix}.$$

$$w_1=\begin{bmatrix} 1 \\ -1 \end{bmatrix}.$$

$$[A-\lambda_2 I]=\begin{bmatrix} -2 & 0 \\ 2 & 0 \end{bmatrix}.$$

$$w_2=\begin{bmatrix} 0 \\ 1 \end{bmatrix}.$$

P, D are

$$P=\begin{bmatrix} 1 & 0 \\ -1 & 1 \end{bmatrix}, \quad D=\begin{bmatrix} 1 & 0 \\ 0 & 3 \end{bmatrix}.$$

Calculate P^{-1}. Use Gauss-Seidel method

$$[P|I]=\left[\begin{array}{cc|cc} 1 & 0 & 1 & 0 \\ -1 & 1 & 0 & 1 \end{array}\right]\sim\left[\begin{array}{cc|cc} 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 1 \end{array}\right].$$

$$P^{-1}=\begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix}.$$

$$\begin{aligned} A^8=PD^8P^{-1} &= \begin{bmatrix} 1 & 0 \\ -1 & 1 \end{bmatrix}\begin{bmatrix} 1^8 & 0 \\ 0 & 3^8 \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 1 & 1 \end{bmatrix} \\ &= \begin{bmatrix} 1 & 0 \\ -1 & 1 \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 3^8 & 3^8 \end{bmatrix} \\ &= \begin{bmatrix} 1 & 0 \\ 3^8-1 & 3^8 \end{bmatrix}=\begin{bmatrix} 1 & 0 \\ 6560 & 6561 \end{bmatrix}. \end{aligned}$$

Question 4. Prove:

a) If λ is an eigenvalue for A then λ^k is an eigenvalue for A^k.

Proof. We shall prove the statements via induction. For $k=1$ we get the trivial case. Now assume that If λ is an eigenvalue for A then λ^m is an eigenvalue for A^m, i.e.

$$A^m x=\lambda^m x$$

For $k=m+1$,

$$\begin{aligned} A^{m+1}x &= A^m A x \\ &= A^m \lambda x \\ &= \lambda A^m x \\ &= \lambda \lambda^m x \\ &= \lambda^{m+1} x. \end{aligned}$$

□

b) If $A^2=A$ and if λ is an eigenvalue for A then $\lambda=0$ or $\lambda=1$.

Proof. If λ is an eigenvalue for A, then

$$Ax=\lambda x.$$

Similarly, based on the previous section, for A^2

$$A^2 x \;=\; \lambda^2 x\,.$$

But since $A^2 = A$, we must have

$$\begin{aligned}(A^2 - A)\,x &= 0\\ \lambda^2 x - \lambda\,x &= 0\\ (\lambda^2 - \lambda)\,x &= 0\end{aligned}$$

which is only generally true for $\lambda = 1$ or $\lambda = 0$, assuming $x \neq \vec{0}$ (which holds by the definition of an eigenvector). $\square$