

Linear Algebra for Chemists — Assignment 8

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Question 1. .

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

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

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

For $n=1$, start from

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

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

$$PP^{-1}APP^{-1} = PD P^{-1}$$

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

Now assume that for $n=k$

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

For $n=k+1$,

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

QED.

- b) Given $A = \begin{bmatrix} 1 & 0 \\ 2 & 3 \end{bmatrix}$, 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 2. Define the Fibonacci sequence as follows:

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

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

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

By 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)

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

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

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

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

Question 3. Perform eigendecomposition on the following:

a)

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

Find eigenvalues.

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

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

Calculate eigenvectors. For $\lambda_1 = 1$,

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

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

The other eigenvalues are not in \mathbb{R} , so the matrix is not diagonalizable over \mathbb{R} .

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 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

$$A x = \lambda x.$$

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). □