$$\boxed{\textbf{Introduction to the Eigenvalue problem}}$$

The eigenvalue problem is a fundamental concept in physical chemistry. At its core, the problem involves finding solutions to the equation,

$$\mathbf{A}\,\mathbf{x} = \lambda\,\mathbf{x}, \tag{1}$$

where $\mathbf{x}$ and λ are known as the **eigenvector** and **eigenvalue** of the matrix $\mathbf{A}$, respectively. λ is a scalar number. Understanding eigenvalues and eigenvectors is essential for analyzing molecular orbitals, vibrational modes, reaction kinectics, and electronic transitions, making it a cornerstone of chemical and physical theory.

1 Computation of eigenvectors and eigenvalues

The computation of $\mathbf{x}$ and λ is carried solving the following homogeneous linear set of equations,

$$\mathbf{A}\,\mathbf{x} - \lambda\,\mathbf{x} = \mathbf{0}, \tag{2}$$

where $\mathbf{x}$ **CANNOT** be a vector with all elements equal to zero. The non-zero solutions to this system of equations can only exist if, the matrix $\mathbf{A} - \lambda\,\mathbf{I}$ is singular,

$$\det\left(\mathbf{A} - \lambda\,\mathbf{I}\right) = \mathbf{0}, \tag{3}$$

where $\mathbf{I}$ is the identity matrix. Eq. 3 is known as the **Secular Equation** and it gives a polynomial in powers of λ. This polynomial is know as the **characteristic polynomial** of $\mathbf{A}$.

The first step into finding the eigenvalues and eigenvectors is to solve the Secular equation. We will first consider the following 2×2 matrix as an example,

$$\mathbf{A} = \begin{bmatrix} -1 & 2 \\ 2 & 2 \end{bmatrix}. \tag{4}$$

giving the following secular equation,

$$\det\left(\mathbf{A} - \lambda\,\mathbf{I}\right) = \begin{bmatrix} -1-\lambda & 2 \\ 2 & 2-\lambda \end{bmatrix} = (-1-\lambda)(2-\lambda) - (2)(2). \tag{5}$$

This give us the following second order equation,

$$\lambda^2 - \lambda - 6 = 0 \tag{6}$$

with the following solutions,

$$\lambda_1 = 3 \quad \text{and} \quad \lambda_2 = -2. \tag{7}$$

λ_1 and λ_2 are the eigenvalues of the matrix $\mathbf{A}$.

The second step is to find the eigenvector for each eigenvalue. Let's first consider λ_1, giving us the following set of questions for $\mathbf{x}_{\lambda_1}$,

$$\left(\mathbf{A} - \lambda_1\,\mathbf{I}\right)\mathbf{x}_{\lambda_1} = \begin{bmatrix} -1-\lambda_1 & 2 \\ 2 & 2-\lambda_1 \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} -1-(3) & 2 \\ 2 & 2-(3) \end{bmatrix}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix} \tag{8}$$

x_1 and x_2 can not be zero, so in order to solve these two linear equations. One approach is to solve x_2 in terms of x_1, giving us,

$$-4x_1 + 2x_2 = 0 \qquad \rightarrow \qquad x_2 = 2x_1 \tag{9}$$
$$-2x_1 + 2x_2 = 0 \qquad \rightarrow \qquad x_2 = 2x_1. \tag{10}$$

From these two equations we can argue that x_2 is twice x_1, because of this, there are many solutions so we can set x_1 equal to a constant, for example, $x_1 = a$. This allow us to define, the eigenvector of λ_1 as,

$$\mathbf{x}_{\lambda_1} = a \begin{bmatrix} 1 \\ 2 \end{bmatrix}. \tag{11}$$

We can do the same procedure for λ_2, giving us the following two equations,

$$x_1 + 2x_2 = 0 \qquad \rightarrow \qquad x_2 = -\frac{x_1}{2} \tag{12}$$
$$2x_1 + 4x_2 = 0 \qquad \rightarrow \qquad x_2 = -\frac{x_1}{2}. \tag{13}$$

where,

$$\mathbf{x}_{\lambda_2} = b \begin{bmatrix} 1 \\ -\frac{1}{2} \end{bmatrix}, \tag{14}$$

and b is other constant similar to a.

The last step is to figure out the values of a and b. We could set them to $a = 1$ and $b = 1$; however, this will make the eigenvectors not normalized, $\mathbf{x}_\lambda^\top \mathbf{x}_\lambda \neq 1$. Using this normalization constrain, $\mathbf{x}_\lambda^\top \mathbf{x}_\lambda = 1$, allows us to find the values of a and b,

$$\mathbf{x}_{\lambda_1}^\top \mathbf{x}_{\lambda_1} = \begin{bmatrix} a & 2a \end{bmatrix}, \begin{bmatrix} a \\ 2a \end{bmatrix} = a^2 + (2a)^2 = a^2(1+4) = 1, \tag{15}$$

if we solve for a, we get $a = \frac{1}{\sqrt{5}}$. The same procedure can be done for $\mathbf{x}_{\lambda_2}$, giving us $b = \frac{2}{\sqrt{5}}$. The eigenvectors of $\mathbf{A}$ are,

$$\mathbf{x}_{\lambda_1} = \begin{bmatrix} \frac{1}{\sqrt{5}} \\ \frac{2}{\sqrt{5}} \end{bmatrix} \quad \text{and} \quad \mathbf{x}_{\lambda_2} = \begin{bmatrix} \frac{2}{\sqrt{5}} \\ -\frac{1}{\sqrt{5}} \end{bmatrix} \tag{16}$$

.

The the eigenvectors can be represented as a matrix $\mathbf{U}$,

$$\mathbf{U} = [\mathbf{x}_{\lambda_1}, \mathbf{x}_{\lambda_2}] = \begin{bmatrix} \frac{1}{\sqrt{5}} & \frac{2}{\sqrt{5}} \\ \frac{2}{\sqrt{5}} & -\frac{1}{\sqrt{5}} \end{bmatrix} \tag{17}$$

. One of the best properties of orthogonal matrices like $\mathbf{U}$ is that $\mathbf{U}^\top$ its the inverse ($\mathbf{U}^{-1}$),

$$\mathbf{U}^{-1}\mathbf{U} = \mathbf{U}^\top \mathbf{U} = \begin{bmatrix} \mathbf{x}_{\lambda_1}^\top \\ \mathbf{x}_{\lambda_2}^\top \end{bmatrix} \begin{bmatrix} \mathbf{x}_{\lambda_1} & \mathbf{x}_{\lambda_2} \end{bmatrix} = \begin{bmatrix} \frac{1}{\sqrt{5}} & \frac{2}{\sqrt{5}} \\ \frac{2}{\sqrt{5}} & -\frac{1}{\sqrt{5}} \end{bmatrix} \begin{bmatrix} \frac{1}{\sqrt{5}} & \frac{2}{\sqrt{5}} \\ \frac{2}{\sqrt{5}} & -\frac{1}{\sqrt{5}} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \mathbf{I} \tag{18}$$

.

As an additional exercise, I encourage you to compute the dot product between $\mathbf{x}_{\lambda_1}$ and $\mathbf{x}_{\lambda_2}$ to show they are orthogonal.

2 Properties of eigenvectors

A matrix $n \times n$ has n eigenpairs, depending on the elements of the matrix there could be eigenvalues that have the same values, meaning they are degenerate. An interesting property is that any linear combination of these eigenvectors that have the same eigenvalue will also be an eigenvector of such matrix. We can easily prove this statement, let's first assume that $\mathbf{x}_1$ and $\mathbf{x}_2$ are both eigenvectors of the matrix $\mathbf{A}$ with the same eigenvalue,

$$\mathbf{A}\,\mathbf{x}_1 = \lambda\,\mathbf{x}_1 \quad \text{and} \quad \mathbf{A}\,\mathbf{x}_2 = \lambda\,\mathbf{x}_2\,. \tag{19}$$

Now, let's define a new eigenvector,

$$\mathbf{x}_{new} = c_1\,\mathbf{x}_1 + c_2\,\mathbf{x}_2, \tag{20}$$

where c_1 and c_2 are the linear combination coefficients. If we plug this into the eigenvalue equation we get the following,

$$\begin{aligned} \mathbf{A}\,\mathbf{x}_{new} &= \mathbf{A}(c_1\,\mathbf{x}_1 + c_2\,\mathbf{x}_2) = c_1\,\mathbf{A}\,\mathbf{x}_1 + c_2\,\mathbf{A}\,\mathbf{x}_2 \\ &= c_1\lambda\,\mathbf{x}_1 + c_2\lambda\,\mathbf{x}_2 = \lambda(c_1\,\mathbf{x}_1 + c_2\,\mathbf{x}_2) = \lambda\,\mathbf{x}_{new}\,. \end{aligned} \tag{21}$$

This proves that $\mathbf{x}_{new}$ is also an eigenvector of $\mathbf{A}$ and has the same eigenvalue of $\mathbf{x}_1$ and $\mathbf{x}_2$.

• Linear combination of eigenvectors that have the same eigenvalue is an eigenvector with the same eigenvalue.

3 Eigenvalues of Hermitian matrices

In quantum chemistry, we commonly work with Hermitian matrices as we will show that their eigenvalues are real numbers. We must remember that a hermitian matrix is define as $\mathbf{A} = \mathbf{A}^\dagger = (\mathbf{A}^*)^\top$. To prove that the eigenvalues of a hermitian matrix are real numbers we need to prove that $\lambda = \lambda^*$, as only real numbers are equal to it's complex conjugate.

$$\mathbf{A}\,\mathbf{x} = \lambda\,\mathbf{x} \qquad (\mathbf{A}\,\mathbf{x})^\dagger = \mathbf{x}^\dagger\,\mathbf{A}^\dagger = \lambda^*\,\mathbf{x}^\dagger \tag{22}$$

$$\text{(left multiply by } \mathbf{x}^\dagger) \quad \mathbf{x}^\dagger\,\mathbf{A}\,\mathbf{x} = \lambda\,\mathbf{x}^\dagger\,\mathbf{x} \qquad \mathbf{x}^\dagger\,\mathbf{A}^\dagger\,\mathbf{x} = \lambda^*\,\mathbf{x}^\dagger\,\mathbf{x} \quad \text{(right multiply by } \mathbf{x}), \tag{23}$$

if we subtract both equations we get,

$$\mathbf{x}^\dagger\,\mathbf{A}\,\mathbf{x} - \mathbf{x}^\dagger\,\mathbf{A}^\dagger\,\mathbf{x} = \lambda\,\mathbf{x}^\dagger\,\mathbf{x} - \lambda^*\,\mathbf{x}^\dagger\,\mathbf{x} \tag{24}$$

$$\mathbf{x}^\dagger(\mathbf{A} - \mathbf{A}^\dagger)\,\mathbf{x} = (\lambda - \lambda^*)\,\mathbf{x}^\dagger\,\mathbf{x}, \tag{25}$$

because we assume $\mathbf{A}$ is a hermitian matrix, $\mathbf{A} - \mathbf{A}^\dagger = 0$, therefore $\lambda = \lambda^*$, which as we mentioned it only happens if λ is a real number.

4 Single Value Decomposition

In class we saw how to compute the inverse of a **square matrix**, $\mathbf{A}\,(n, n)$. However, what happens when we want to invert a rectangular matrix, meaning a matrix that has more rows than columns or viceversa, more columns than rows? Linear equations as you know could also describe problems where have either more points (rows) than features (columns), ir vice versa more features (columns) than points (rows). The case where the number of points is bigger than the number of columns is known as **Overdetermined**.

Because $\mathbf{A}$ is not a square matrix,

$$\mathbf{A} = \begin{bmatrix} a_{1,1} & a_{1,2} & \cdots & a_{1,m} \\ a_{2,1} & a_{2,2} & \cdots & a_{2,m} \\ \vdots & \vdots & \ddots & \vdots \\ a_{n-1,1} & a_{n-1,2} & \cdots & a_{n-1,m} \\ a_{n,1} & a_{n,2} & \cdots & a_{n,m} \end{bmatrix}, \tag{26}$$

where $n > m$.
We can approximate the inverse of these matrix using Singular Value Decomposition (SVD) `https://sthalles.github.io/svd-for-regression/`.

The SVD of a matrix $\mathbf{A}$ is given by

$$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^T \tag{27}$$

where $\mathbf{U}$ and $\mathbf{V}^T$ are orthogonal matrices,

$$\mathbf{U}^T\mathbf{U} = \mathbf{I} \tag{28}$$
$$\mathbf{V}^T\mathbf{V} = \mathbf{I}, \tag{29}$$

and $\mathbf{\Sigma}$ is a diagonal matrix with non-negative real numbers on the diagonal.

Due to the shortness of the course we will not properly review SVDs, but is one of the main building blocks in scientific computing. Let's review SVD under the scope of linear equations. The idea if SVD is to approximate the inverse of $\mathbf{A}$.

$$\mathbf{A}\mathbf{x} = \mathbf{b} \tag{30}$$
$$\underbrace{\left(\mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top\right)}_{\mathbf{A}}\mathbf{x} = \mathbf{b} \tag{31}$$
$$\left(\mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top\right)^{-1}\left(\mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top\right)\mathbf{x} = \left(\mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top\right)^{-1}\mathbf{b} \tag{32}$$
$$\mathbf{V}\mathbf{\Sigma}^{-1}\mathbf{U}^\top\mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top\mathbf{x} = \left(\mathbf{V}\mathbf{\Sigma}^{-1}\mathbf{U}^\top\right)\mathbf{b}, \tag{33}$$

we can cancel some terms, using the orthogonality property of $\mathbf{U}$ and $\mathbf{V}$, giving us,

$$\mathbf{x} = \mathbf{V}\mathbf{\Sigma}^{-1}\mathbf{U}^\top\mathbf{b} \tag{34}$$
$$\mathbf{x} = \mathbf{A}^+\mathbf{b}, \tag{35}$$

where $\mathbf{A}^+$ is known as the **pseudo** inverse of $\mathbf{A}$; $\mathbf{A}^+\mathbf{A} \approx \mathbf{I}$.

For linear models, we can use SVD assuming $\mathbf{x}$ is $\mathbf{w}$ (parameters), $\mathbf{A}$ is $\mathbf{X}$ or $\Phi(\mathbf{X})$ (training data matrix), and $\mathbf{b}$ is $\mathbf{y}$.

Extra: $\left(\mathbf{U}\mathbf{\Sigma}\mathbf{V}^\top\right)^{-1} = \left(\mathbf{V}\mathbf{\Sigma}^{-1}\mathbf{U}^\top\right)$ is explained in Eq. 223 of The Matrix Cookbook

You can get the SVD of any matrix in Numpy using the following code,

```python
import numpy as np

X = np.random.rand(10, 3) # Rectangular matrix: 10 rows, 3 columns
U, S, Vt = np.linalg.svd(X, full_matrices=False) # Perform SVD on X
```

5 Coupled Linear Ordinary Differential Equations

In this section, we will show how the eigenvalue problem can be use in the computation of ordinary differential equations (ODEs). Let's assume the following time ODE,

$$\frac{d\,\mathbf{x}}{dt} = \mathbf{A}\,\mathbf{x} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ \vdots & & \cdots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}, \tag{36}$$

if the off-diagonal elements of $\mathbf{A}$ where zero, we will have $n-$decoupled time differential equations of the form $\frac{dx_i}{dt} = a_{ii}x_i$. Before we proceed, let's remember the solution of this style of differential equation, $x_i(t) = e^{a_{ii}t}x_i(t_0)$. Inspired from this solution form, we seek a general solution for Eq. 36 of a similar form. The general solution of these coupled linear ODEs are,

$$\mathbf{x}(t) = e^{\mathbf{A}\,t}\,\mathbf{x}(t_0) = \sum_i c_i e^{\lambda_i t}\,\mathbf{v}_i, \tag{37}$$

where $\mathbf{v}_i$ and λ_i are unknown vectors and numbers.

Inspired by the general form solution, Eq. 37, we can first start with a possible guess $\tilde{\mathbf{x}}(t) = \mathbf{v}\,e^{\lambda t}$,

$$\frac{d\tilde{\mathbf{x}}}{dt} = \frac{d\,\mathbf{v}\,e^{\lambda t}}{dt} = \lambda\,\mathbf{v}\,e^{\lambda t} = \mathbf{A}\,\underbrace{\mathbf{v}\,e^{\lambda t}}_{\tilde{\mathbf{x}}}. \tag{38}$$

We can cancel the $e^{\lambda t}$ term, getting,

$$\mathbf{A}\,\mathbf{v} = \lambda\,\mathbf{v}\,. \tag{39}$$

This is another eigenvalue problem. To solve it, we can follow the steps described in Section 1.

1. Solve the Secular equation, $\det(\mathbf{A} - \lambda\,\mathbf{I}) = 0$ and find the eigenvalues $\{\lambda_i\}_{i=1}^{n}$.
2. For each eigenvalue λ_i, solve $(\mathbf{A} - \lambda_i\,\mathbf{I})\,\mathbf{v} = 0$.

We will have n solutions, and we can not rule out any of them, so we can construct a general solution using all $n-$eigenpairs,

$$\mathbf{x}(t) = \sum_i c_i e^{\lambda_i t}\,\mathbf{v}_i, \tag{40}$$

where the c_i coefficients can be found using the **boundary conditions** of the problem. The most common of the types of boundary conditions is the initial value of $\mathbf{x}$ at $t = 0$. This means that Eq. 40 must be the same for the known values of $\mathbf{x}(t_0)$,

$$\mathbf{x}(t_0) = \sum_i c_i\,\mathbf{v}_i, \tag{41}$$

in vector representation we have,

$$\underbrace{\begin{bmatrix} x_1(t_0) \\ x_2(t_0) \\ \vdots \\ x_n(t_0) \end{bmatrix}}_{\mathbf{x}(t_0)} = \sum_i c_i\,\mathbf{v}_i = \underbrace{\begin{bmatrix} \mathbf{v}_1, & \mathbf{v}_2, & \cdots, & \mathbf{v}_n \end{bmatrix}}_{\mathbf{U}} \underbrace{\begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{bmatrix}}_{\mathbf{c}}. \tag{42}$$

This equation is another linear set of equations where the unknown is the vector of linear coefficients c_is. There is no reason to do solve for $\mathbf{c}$ by inverting the matrix $\mathbf{U}$; $\mathbf{c} = \mathbf{U}^{-1}\,\mathbf{x}(t_0)$. $\mathbf{U}$ is an orthogonal matrix, $\mathbf{U}^\top = \mathbf{U}^{-1}$, as $\mathbf{U}^\top\,\mathbf{U} = \mathbf{I}$. Therefore,

$$\underbrace{\begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{bmatrix}}_{\mathbf{c}} = \underbrace{\begin{bmatrix} \mathbf{v}_1^\top \\ \mathbf{v}_n^\top \\ \vdots \\ \mathbf{v}_n^\top \end{bmatrix}}_{\mathbf{U}^\top} \underbrace{\begin{bmatrix} x_1(t_0) \\ x_2(t_0) \\ \vdots \\ x_n(t_0) \end{bmatrix}}_{\mathbf{x}(t_0)} \tag{43}$$

The last step is simply use the values of $\mathbf{c}$ in Eq. 40.

5.1 Matrix exponential

The solution of Eq. 36, can be written in terms of the **matrix exponential**, $e^{\mathbf{A}\,t}$. This does not mean we simply take the exponential of each element of $\mathbf{A}$. The matrix exponential can be rewritten in terms of the eigenvalue basis,

$$e^{\mathbf{A}\,t} = \mathbf{U}\,e^{\Lambda\,t}\,\mathbf{U}^\top, \tag{44}$$

where $\mathbf{U}$ and Λ are the matrix with all the eigenvectors and eigenvectors, respectively,

$$\mathbf{U} = \begin{bmatrix} \mathbf{v}_1, & \mathbf{v}_2, & \cdots, & \mathbf{v}_n \end{bmatrix} \quad \text{and} \quad \Lambda = \begin{bmatrix} \lambda_1 & 0, & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \lambda_i & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{bmatrix}. \tag{45}$$

To prove Eq. 44, we first need to dive a little deeper in the matrix eigenvalue problem. So far we know that for each eigenpair, $\mathbf{A}\,\mathbf{x}_i = \lambda_i\,\mathbf{x}_i$. For all eigenpairs we can rewrite the eigenvalue equation as,

$$\mathbf{A}\,\mathbf{U} = \mathbf{U}\,\Lambda \tag{46}$$

$$\mathbf{A}\begin{bmatrix} \mathbf{v}_1, & \mathbf{v}_2, & \cdots, & \mathbf{v}_n \end{bmatrix} = \begin{bmatrix} \mathbf{v}_1, & \mathbf{v}_2, & \cdots, & \mathbf{v}_n \end{bmatrix} \begin{bmatrix} \lambda_1 & 0, & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \lambda_i & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{bmatrix} \tag{47}$$

$$\begin{bmatrix} \mathbf{A}\,\mathbf{v}_1, & \mathbf{A}\,\mathbf{v}_2, & \cdots, & \mathbf{A}\,\mathbf{v}_n \end{bmatrix} = \begin{bmatrix} \lambda_1\,\mathbf{v}_1, & \lambda_2\,\mathbf{v}_2, & \cdots, & \lambda_n\,\mathbf{v}_n \end{bmatrix}. \tag{48}$$

Exercise: Prove Eq. 46 and also show that, $\begin{bmatrix} \lambda_1\,\mathbf{v}_1, & \lambda_2\,\mathbf{v}_2, & \cdots, & \lambda_n\,\mathbf{v}_n \end{bmatrix} \neq \Lambda\,\mathbf{U}$.

Using Eq. 46 we can define a relation between $\mathbf{A}$ and all the eigenpairs,

$$\mathbf{A}\underbrace{\mathbf{U}\,\mathbf{U}^\top}_{\mathbf{I}} = \mathbf{U}\,\Lambda\,\mathbf{U}^\top \quad \text{right multiply by } \mathbf{U}^\top \tag{49}$$

$$\mathbf{A} = \mathbf{U}\,\Lambda\,\mathbf{U}^\top. \tag{50}$$

Eq. 50 tells us that $\mathbf{A}$ can be reconstructed using all the eigenvalues and eigenvectors. This is similar to the SVD decomposition we saw when doing linear equations. We can use only some of the eigenpairs and not all to reconstruct $\mathbf{A}$,

$$\mathbf{A} \approx \mathbf{A}_{\text{rec}} = \mathbf{U}_m\,\Lambda_m\,\mathbf{U}^\top{}_m \tag{51}$$

$$= \underbrace{\begin{bmatrix} \mathbf{v}_1, & \mathbf{v}_2, & \cdots, & \mathbf{v}_m \end{bmatrix}}_{(n,m)} \underbrace{\begin{bmatrix} \lambda_1 & 0, & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \lambda_i & \vdots \\ 0 & 0 & \cdots & \lambda_m \end{bmatrix}}_{(m,m)} \underbrace{\begin{bmatrix} \mathbf{v}_1^\top \\ \mathbf{v}_2^\top \\ \vdots \\ \mathbf{v}_m^\top \end{bmatrix}}_{(m,n)}. \tag{52}$$

Let us go back to the matrix exponential problem but now using this new relation. First, let's do the series expansion of the exponential function,

$$
\begin{aligned}
e^{\mathbf{A}\,t} &= \sum_{k=0}^{\infty} \frac{(\mathbf{A}\,t)^k}{k!} = \left(\mathbf{I} + \mathbf{A}\,t + \frac{(\mathbf{A}\,t)^2}{2!} + \frac{(\mathbf{A}\,t)^3}{3!} + \cdots\right) && (53)\\
&= \left(\mathbf{I} + \mathbf{A}\,t + \frac{t^2}{2!}\,\mathbf{A}\,\mathbf{A} + \frac{t^3}{3!}\,\mathbf{A}\,\mathbf{A}\,\mathbf{A} + \cdots\right), && (54)
\end{aligned}
$$

Let's replace $\mathbf{A}$ with Eq. 50,

$$
e^{\mathbf{A}\,t} = \left(\mathbf{I} + \underbrace{\left(\mathbf{U}\,\Lambda\,\mathbf{U}^\top\right)}_{\mathbf{A}} t + \frac{t^2}{2!}\left(\mathbf{U}\,\Lambda\,\mathbf{U}^\top\right)\left(\mathbf{U}\,\Lambda\,\mathbf{U}^\top\right) + \frac{t^3}{3!}\left(\mathbf{U}\,\Lambda\,\mathbf{U}^\top\right)\left(\mathbf{U}\,\Lambda\,\mathbf{U}^\top\right)\left(\mathbf{U}\,\Lambda\,\mathbf{U}^\top\right) + \cdots\right), \quad (55)
$$

this expansion can be "cleaned" using the orthogonality property of $\mathbf{U}$, meaning $\mathbf{U}^\top\,\mathbf{U} = \mathbf{I}$,

$$
\begin{aligned}
e^{\mathbf{A}\,t} &= \left(\mathbf{I} + \mathbf{U}\,\Lambda\,\mathbf{U}^\top\,t + \frac{t^2}{2!}\,\mathbf{U}\,\Lambda\underbrace{\mathbf{U}^\top\,\mathbf{U}}_{\mathbf{I}}\Lambda\,\mathbf{U}^\top + \frac{t^3}{3!}\,\mathbf{U}\,\Lambda\underbrace{\mathbf{U}^\top\,\mathbf{U}}_{\mathbf{I}}\Lambda\underbrace{\mathbf{U}^\top\,\mathbf{U}}_{\mathbf{I}}\Lambda\,\mathbf{U}^\top + \cdots\right)\\
&= \left(\mathbf{I} + \mathbf{U}\,\Lambda\,\mathbf{U}^\top\,t + \frac{t^2}{2!}\,\mathbf{U}\,\Lambda\,\Lambda\,\mathbf{U}^\top + \frac{t^3}{3!}\,\mathbf{U}\,\Lambda\,\Lambda\,\Lambda\,\mathbf{U}^\top + \cdots\right)\\
&= \mathbf{U}\left(\mathbf{I} + \Lambda\,t + \frac{(\Lambda\,t)^2}{2!} + \frac{(\Lambda\,t)^3}{3!} + \cdots\right)\mathbf{U}^\top = \mathbf{U}\left(\sum_{k=0}^{\infty}\frac{(\Lambda\,t)^k}{k!}\right)\mathbf{U}^\top\\
&= \mathbf{U}\,e^{\Lambda\,t}\,\mathbf{U}^\top, && (56)
\end{aligned}
$$

where

$$
e^{\Lambda\,t} = \begin{bmatrix} e^{\lambda_1 t} & 0, & \cdots & 0\\ 0 & e^{\lambda_2 t} & \cdots & 0\\ \vdots & \vdots & e^{\lambda_i t} & \vdots\\ 0 & 0 & \cdots & e^{\lambda_n t} \end{bmatrix} \quad (57)
$$

Since Λ is a diagonal matrix, any power of the eigenvalues matrix is simply each eigenvalue raised to that specific power,

$$
\begin{aligned}
\Lambda^p &= \begin{bmatrix} \lambda_1 & 0, & \cdots & 0\\ 0 & \lambda_2 & \cdots & 0\\ \vdots & \vdots & \lambda_i & \vdots\\ 0 & 0 & \cdots & \lambda_m \end{bmatrix}\begin{bmatrix} \lambda_1 & 0, & \cdots & 0\\ 0 & \lambda_2 & \cdots & 0\\ \vdots & \vdots & \lambda_i & \vdots\\ 0 & 0 & \cdots & \lambda_m \end{bmatrix}\cdots\begin{bmatrix} \lambda_1 & 0, & \cdots & 0\\ 0 & \lambda_2 & \cdots & 0\\ \vdots & \vdots & \lambda_i & \vdots\\ 0 & 0 & \cdots & \lambda_m \end{bmatrix}\\
&= \begin{bmatrix} \lambda_1^p & 0, & \cdots & 0\\ 0 & \lambda_2^p & \cdots & 0\\ \vdots & \vdots & \lambda_i^p & \vdots\\ 0 & 0 & \cdots & \lambda_m^p \end{bmatrix} && (58)
\end{aligned}
$$

Excercise: Show that $\sum_{k=0}^{\infty}\frac{(\Lambda\,t)^k}{k!} = \sum_{k=0}^{\infty}\frac{t^k}{k!}(\Lambda)^k$.

The next step is to simply plug in, Eq. 56 in Eq. 37,

$$
\mathbf{x}(t) = e^{\mathbf{A}\,t}\,\mathbf{x}(t_0) = \mathbf{U}\,e^{\Lambda\,t}\underbrace{\mathbf{U}^\top\,\mathbf{x}(t_0)}_{\mathbf{c}} = \mathbf{U}\,e^{\Lambda\,t}\,\mathbf{c}, \quad (59)
$$

if we pay close attention, we can see that there is a similarity with Eq. 43, where we solve the linear equations for the vector $\mathbf{c}$. The last step is to show that this can be rewritten as a sum of vectors,

$$\begin{aligned}
\mathbf{x}(t) &= \mathbf{U}\,e^{\Lambda\,t}\,\mathbf{c} = \begin{bmatrix}\mathbf{v}_1, & \mathbf{v}_2, & \cdots, & \mathbf{v}_n\end{bmatrix} \begin{bmatrix} e^{\lambda_1 t} & 0, & \cdots & 0 \\ 0 & e^{\lambda_2 t} & \cdots & 0 \\ \vdots & \vdots & e^{\lambda_i t} & \vdots \\ 0 & 0 & \cdots & e^{\lambda_n t} \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \end{bmatrix} \\
&= \begin{bmatrix}\mathbf{v}_1, & \mathbf{v}_2, & \cdots, & \mathbf{v}_n\end{bmatrix} \begin{bmatrix} c_1 e^{\lambda_1 t} \\ c_2 e^{\lambda_2 t} \\ \vdots \\ c_n e^{\lambda_n t} \end{bmatrix} = \sum_i^n c_i e^{\lambda_i t}\,\mathbf{v}_i, \qquad (60)
\end{aligned}$$

where in the last step it ”look” like a dot product.