Eigenvalues & Eigenvectors

In general, the operation of a matrix on a vector

$$\underline{\underline{A}} \cdot \vec{v} = \vec{w}$$

results in a <u>transformed</u> vector ($\vec{w}$) which has been scaled, rotated, skewed, smashed, projected, etc.

For example:

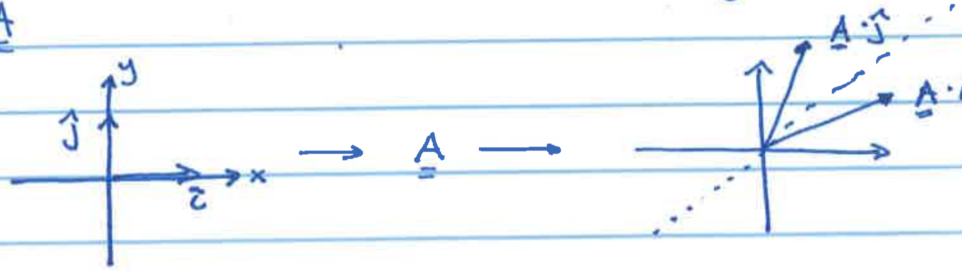
$$\underline{\underline{A}} = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$$

takes the unitvectors $\hat{\imath}$ & $\hat{\jmath}$ to:

$$\underline{\underline{A}} \cdot \hat{\imath} = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 2 \\ 1 \end{pmatrix}$$

$$\underline{\underline{A}} \cdot \hat{\jmath} = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$$

Note that x & y get treated in opposite ways
As a result there's a bit of symmetry to the operation of $\underline{\underline{A}}$



The operation of $\underline{\underline{A}}$ is symmetric along $y = x$
vectors get bent toward this line.

Consider what happens when we take a vector that is <u>on</u> this line $\vec{u} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

$$\underline{\underline{A}} \cdot \vec{u} = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 2+1 \\ 1+2 \end{pmatrix} = \begin{pmatrix} 3 \\ 3 \end{pmatrix} = 3\vec{u}$$

For this special vector $\underline{\underline{A}}$ acts like a scaling operation. It also works on multiples of $\vec{u}$:

$$\underline{\underline{A}} \cdot \begin{pmatrix} 2 \\ 2 \end{pmatrix} = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}\begin{pmatrix} 2 \\ 2 \end{pmatrix} = \begin{pmatrix} 6 \\ 6 \end{pmatrix} = 3\begin{pmatrix} 2 \\ 2 \end{pmatrix}$$

More generally

$$\underline{\underline{A}}\left[c\begin{pmatrix} 1 \\ 1 \end{pmatrix}\right] = c\,\underline{\underline{A}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = 3c\begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$\underline{\underline{A}}$ has another one of these special vectors $\vec{v} = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$

$$\underline{\underline{A}} \cdot \vec{v} = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}\begin{pmatrix} 1 \\ -1 \end{pmatrix} = \begin{pmatrix} 2-1 \\ 1-2 \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \vec{v}$$

For any matrix, we can express the problem of finding these special vectors as

$$\underline{\underline{A}}\,\vec{v} = \lambda \vec{v}$$

where λ is a <u>constant</u>. We call these special vectors <u>eigenvectors</u> and the associated values λ are called <u>eigenvalues</u>. Eigen means "self" or "own" in german, and they are special self-vectors for each matrix.

Eigenvalues & Eigenvectors are <u>spectacularly</u> <u>useful</u>

- They tell you about the symmetries of a matrix operation $\left[\begin{pmatrix} 1 \\ 1 \end{pmatrix} \text{ \& } \begin{pmatrix} 1 \\ -1 \end{pmatrix}\right.$ tell you about the stretching axis of $\left.\underline{\underline{A}}\right]$

- They let you <u>diagonalize</u> a matrix to learn about (~~the~~ and simplify other} operations]

(Later we'll cover how we can go from

$$\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \longrightarrow \begin{pmatrix} 3 & 0 \\ 0 & 1 \end{pmatrix}$$

- Eigenvalue equations appear everywhere in Quantum Mechanics: The Schrodinger wave equation can be written as one:

$$H\psi = E\psi$$

allowed behaviors of the system (eigen functions)

associated energies of states

Hamiltonian or total energy operator.

Matrix Eigenvalues

$$\underline{\underline{A}}\,\vec{v} = \lambda\,\vec{v}$$

We can use the identity matrix $\underline{\underline{I}}\,\vec{v} = \vec{v}$ to rearrange

$$\underline{\underline{A}}\cdot\vec{v} = \lambda\,\underline{\underline{I}}\cdot\vec{v}$$

$$\underline{\underline{A}}\cdot\vec{v} - \lambda\,\underline{\underline{I}}\cdot\vec{v} = 0$$

$$(\underline{\underline{A}} - \lambda\underline{\underline{I}})\cdot\vec{v} = 0$$

If we write out $\underline{\underline{A}}$ in terms of its components

$$\underline{\underline{A}} = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & & & \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix}$$

then we get

$$\underline{\underline{A}} - \lambda \underline{\underline{I}} = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & & & \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} - \begin{pmatrix} \lambda & 0 & \cdots & 0 \\ 0 & \lambda & \cdots & 0 \\ 0 & & & \\ \vdots & & & \\ 0 & \cdots & & \lambda \end{pmatrix}$$

In otherwords, we subtract λ from each diagonal component.

$$\begin{pmatrix} a_{11}-\lambda & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22}-\lambda & \cdots & a_{2n} \\ \vdots & & & \\ a_{n1} & \cdots & & a_{nn}-\lambda \end{pmatrix} \cdot \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_n \end{pmatrix} = 0$$

This is exactly the type of problem we covered in linear systems, and a non-trivial solution requires:

$$\det(\underline{\underline{A}} - \lambda \underline{\underline{I}}) = 0$$

Characteristic Equation

The determinant results in what is called a characteristic or secular equation for $\underline{\underline{A}}$ where the roots are eigenvalues:

Here's our example matrix:

$$\det(A - \lambda I) = 0$$

$$\det\left(\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} - \lambda \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right) = 0$$

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

$$(2-\lambda)^2 - 1 = 0$$

So
$$\lambda^2 - 4\lambda + 4 - 1 = 0$$
$$\lambda^2 - 4\lambda + 3 = 0$$

$$(\lambda - 3)(\lambda - 1) = 0$$

This tells us that $\lambda = 3$ or $\lambda = 1$

this is the procedure for finding eigenvalues.

To find the eigenvectors

We go back to:

$$(\underline{A} - \lambda \underline{I})\vec{v} = 0$$

and substitute in each of the values of λ (one at a time)

For $\lambda = 3$ we'd have

$$\left[\begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} - 3\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\right]\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = 0$$

$$\begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = 0$$

$$\left.\begin{aligned} -v_1 + v_2 &= 0 \\ v_1 - v_2 &= 0 \end{aligned}\right] \rightarrow \text{both tell us that } v_1 = v_2$$

Let's do a 3x3 example:

$$\underline{A} = \begin{pmatrix} 1 & 2\sqrt{3} & -\sqrt{3} \\ -\sqrt{3} & 2 & 3 \\ 2\sqrt{3} & 0 & 2 \end{pmatrix}$$

Solve for λ first:

$$\begin{vmatrix} 1-\lambda & 2\sqrt{3} & -\sqrt{3} \\ -\sqrt{3} & 2-\lambda & 3 \\ 2\sqrt{3} & 0 & 2-\lambda \end{vmatrix} = 0$$

$$2\sqrt{3}\begin{vmatrix} 2\sqrt{3} & -\sqrt{3} \\ 2-\lambda & 3 \end{vmatrix} + (2-\lambda)\begin{vmatrix} 1-\lambda & 2\sqrt{3} \\ -\sqrt{3} & 2-\lambda \end{vmatrix} = 0$$

$$2\sqrt{3}\left(6\sqrt{3} - 2\sqrt{3} + \sqrt{3}\lambda\right) + (2-\lambda)\left((1-\lambda)(2-\lambda) + 6\right) = 0$$

$$36 + 12 - 6\lambda + (2-\lambda)(\lambda^2 - 3\lambda + 8) = 0$$

$$-\lambda^3 + 5\lambda^2 - 20\lambda + 64 = 0$$

$$(\lambda - 4)(\lambda^2 - \lambda + 16) = 0$$

one of the roots is easy
the others, not so much.

$\lambda = 4$, to find associated eigenvector:

$$\begin{pmatrix} -3 & 2\sqrt{3} & -\sqrt{3} \\ -\sqrt{3} & -2 & 3 \\ 2\sqrt{3} & 0 & -2 \end{pmatrix}\begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} = 0$$

And solve the linear system: $v_1 = 1$
$v_2 = \sqrt{3}$
$v_3 = \sqrt{3}$

Check:

$$\begin{pmatrix} 1 & 2\sqrt{3} & -\sqrt{3} \\ -\sqrt{3} & 2 & 3 \\ 2\sqrt{3} & 0 & 2 \end{pmatrix}\begin{pmatrix} 1 \\ \sqrt{3} \\ \sqrt{3} \end{pmatrix} = \begin{pmatrix} 1+6-3 \\ -\sqrt{3}+2\sqrt{3}+3\sqrt{3} \\ 2\sqrt{3}+2\sqrt{3} \end{pmatrix}$$

$$= \begin{pmatrix} 4 \\ 4\sqrt{3} \\ 4\sqrt{3} \end{pmatrix}$$

$$= 4\begin{pmatrix} 1 \\ \sqrt{3} \\ \sqrt{3} \end{pmatrix}$$

Applications of Eigenvalues & Eigenvectors

Kinetics
$$A \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} B \xrightarrow{k_2} C$$

Mechanisms give rise to coupled differential equations:

$$\frac{dA}{dt} = -k_1 A + k_{-1} B$$

$$\frac{dB}{dt} = k_1 A - k_{-1} B - k_2 B$$

$$\frac{dC}{dt} = k_2 B$$

If we make a column vector of concentrations: $\begin{pmatrix} A \\ B \\ C \end{pmatrix}$

we can write these kinetic equations in a matrix form:

$$d/dt \begin{pmatrix} A \\ B \\ C \end{pmatrix} = \begin{pmatrix} -k_1 & k_{-1} & 0 \\ k_1 & -(k_{-1}+k_2) & 0 \\ 0 & k_2 & 0 \end{pmatrix} \begin{pmatrix} A \\ B \\ C \end{pmatrix}$$

Suppose we are able to measure the rates of each step separately:

$$k_1 = 2$$
$$k_{-1} = 5$$
$$k_2 = 1$$

This gives the matrix:

$$\begin{pmatrix} -2 & 5 & 0 \\ 2 & -6 & 0 \\ 0 & 1 & 0 \end{pmatrix}$$

One way to solve coupled linear equations is to get the <u>eigenvalues</u> & <u>eigenvectors</u> for this matrix:

$$\det\left(\underline{A}-\lambda\underline{I}\right)=0 \hookrightarrow \begin{vmatrix} -2-\lambda & 5 & 0 \\ 2 & -6-\lambda & 0 \\ 0 & 1 & -\lambda \end{vmatrix} = 0$$

$$-\lambda\left[(-2-\lambda)(-6-\lambda) - 5\cdot 2\right] = 0$$

$$\lambda\left((12+8\lambda+\lambda^2)-10\right) = 0$$

$$\lambda\underbrace{\left(\lambda^2+8\lambda+2\right)}_{\Rightarrow\ \lambda=-4\pm\sqrt{14}} = 0$$

$$\lambda = 0$$

Let's go through the mess of solving the eigenvectors too:

For $\lambda = -4+\sqrt{14}$

$$\begin{pmatrix} -2-(-4+\sqrt{14}) & 5 & 0 \\ 2 & -6-(-4+\sqrt{14}) & 0 \\ 0 & 1 & -(4+\sqrt{14}) \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = 0$$

$$\begin{pmatrix} 2-\sqrt{14} & 5 & 0 \\ 2 & -2-\sqrt{14} & 0 \\ 0 & 1 & 4-\sqrt{14} \end{pmatrix}\begin{pmatrix} a \\ b \\ c \end{pmatrix} = 0$$

$$\begin{aligned} (2-\sqrt{14})a + 5b &= 0 \\ 2a + (-2-\sqrt{14})b &= 0 \\ b + (4-\sqrt{14})c &= 0 \end{aligned}$$

Set $c=1$, and:

$$b = -(4-\sqrt{14})$$

$$2a + (-2-\sqrt{14})\,b = 0$$

$$2a = -(-2-\sqrt{14})(-4+\sqrt{14})$$
$$= -8 - 4\sqrt{14} + 2\sqrt{14} + 14$$
$$= 6 - 2\sqrt{14}$$

$$a = 3 - \sqrt{14}$$

$$\vec{V}_1 = \begin{pmatrix} 3-\sqrt{14} \\ -4+\sqrt{14} \\ 1 \end{pmatrix} \qquad \lambda_1 = -4+\sqrt{14}$$

The others are:

$$\vec{V}_2 = \begin{pmatrix} 3+\sqrt{14} \\ -4-\sqrt{14} \\ 1 \end{pmatrix} \qquad \lambda_2 = -4-\sqrt{14}$$

$$\vec{V}_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \qquad \lambda_3 = 0$$

But what do these tell us about our kinetics problem?

Consider the last eigenvalue:

$$\frac{d}{dt}\begin{pmatrix} A \\ B \\ C \end{pmatrix} = \underline{\underline{M}}\begin{pmatrix} A \\ B \\ C \end{pmatrix}$$

If <u>only</u> C is present, $\begin{pmatrix} A \\ B \\ C \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$

That vector is an eigenvector of $\underline{\underline{M}}$

$$\underline{\underline{M}}\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = 0\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = 0$$

So:

$$\frac{d}{dt}\begin{pmatrix}0\\0\\1\end{pmatrix} = \underline{M}\begin{pmatrix}0\\0\\1\end{pmatrix} = 0\begin{pmatrix}0\\0\\1\end{pmatrix} = 0$$

That is, if we start with only $\underline{C}$, there's no change in any of the concentrations.

The other eigenvectors are more interesting:

$$\vec{v}_1 = \begin{pmatrix}3-\sqrt{14}\\-4+\sqrt{14}\\1\end{pmatrix} \qquad \lambda_1 = -4+\sqrt{14}$$

$$\frac{d}{dt}\begin{pmatrix}3-\sqrt{14}\\-4+\sqrt{14}\\1\end{pmatrix} = \underline{M}\begin{pmatrix}3-\sqrt{14}\\-4+\sqrt{14}\\1\end{pmatrix} = -(4-\sqrt{14})\begin{pmatrix}3-\sqrt{14}\\-4+\sqrt{14}\\1\end{pmatrix}$$

If you have concentrations in the ratios:

$$A : B : C = 3-\sqrt{14} : -4+\sqrt{14} : 1$$

then the differential equation is easy to solve

$$\frac{d}{dt}\begin{pmatrix}3-\sqrt{14}\\-4+\sqrt{14}\\1\end{pmatrix} x = -(4-\sqrt{14})\begin{pmatrix}3-\sqrt{14}\\-4+\sqrt{14}\\1\end{pmatrix} x$$

Or:

$$x = c_1 e^{-(4-\sqrt{14})t}$$

Likewise:

$$\frac{d}{dt}\begin{pmatrix}3+\sqrt{14}\\-4-\sqrt{14}\\1\end{pmatrix} y = -(4+\sqrt{14})\begin{pmatrix}3+\sqrt{14}\\-4-\sqrt{14}\\1\end{pmatrix} y$$

$$y = c_2 e^{-(4+\sqrt{14})t}$$

The 3 eigenvectors represent 3 <u>steady states</u> where the <u>relative concentrations</u> don't change over time.

Here's the <u>big idea</u>:

<u>Any</u> concentrations can be expressed as a combination of the 3 eigenstates, and once we know the eigenvectors & eigenvalues, we know the future concentrations of <u>any</u> state:

$A(0) = 1$
$B(0) = 0$ ← start with <u>only</u> A
$C(0) = 0$

$$\begin{pmatrix} A(0) \\ B(0) \\ C(0) \end{pmatrix} = c_1(0) \begin{pmatrix} 3-\sqrt{14} \\ -4+\sqrt{14} \\ 1 \end{pmatrix} + c_2(0) \begin{pmatrix} 3+\sqrt{14} \\ -4-\sqrt{14} \\ 1 \end{pmatrix} + c_3(0) \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

Solving this:

$$c_1(0) = -1.0345$$
$$c_2(0) = 0.0345$$
$$c_3(0) = 1$$

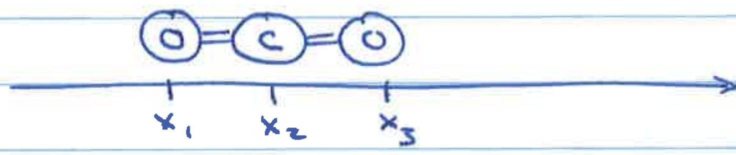
$$\begin{pmatrix} A(t) \\ B(t) \\ C(t) \end{pmatrix} = c_1(t)\,\vec{V}_1 + c_2(t)\,\vec{V}_2 + c_3(t)\,\vec{V}_3$$

With

$$c_1(t) = c_1(0)\, e^{-(4-\sqrt{14})t}$$
$$c_2(t) = c_2(0)\, e^{-(4+\sqrt{14})t}$$
$$c_3(t) = c_3(0)\, e^{0t} = c_3(0)$$

$$\begin{pmatrix} A \\ B \\ C \end{pmatrix} = -1.0345 e^{-(4-\sqrt{14})t} \begin{pmatrix} 3-\sqrt{14} \\ -4+\sqrt{14} \\ 1 \end{pmatrix} + 0.0345 e^{-(4+\sqrt{14})t} \begin{pmatrix} 3+\sqrt{14} \\ -4-\sqrt{14} \\ 1 \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

Application #2 : Molecular Vibrations:



$$V_1 = \frac{1}{2} k \left(x_2 - x_1 - l_0 \right)^2$$

$$V_2 = \frac{1}{2} k \left(x_3 - x_2 - l_0 \right)^2$$

Harmonic Springs

$$F_1 = \frac{-\partial V}{\partial x_1} = +k \left(x_2 - x_1 - l_0 \right)$$

$$F_2 = \frac{-\partial V}{\partial x_2} = -k \left(x_2 - x_1 - l_0 \right) + k \left(x_3 - x_2 - l_0 \right)$$

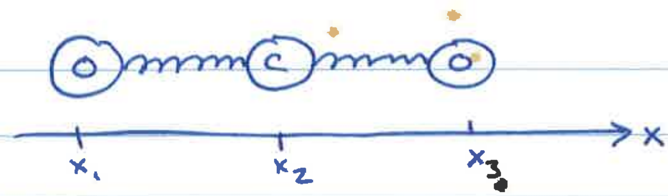
$$F_3 = \frac{-\partial V}{\partial x_3} = -k \left(x_3 - x_2 - l_0 \right)$$

$$F_1 = m_1 a_1 = m_1 \frac{\partial^2 x_1}{\partial t^2}$$

$$m_1 \frac{\partial^2 x_1}{\partial t^2} = k \left(x_2 - x_1 - l_0 \right)$$

$$m_2 \frac{\partial^2 x_2}{\partial t^2} = k \left(x_3 - 2x_2 + x_1 \right)$$

$$m_3 \frac{\partial^2 x_3}{\partial t^2} = -k \left(x_3 - x_2 - l_0 \right)$$



Potential Energy $= \frac{1}{2}k(x_2 - x_1 - l_0)^2 + \frac{1}{2}k(x_3 - x_2 - l_0)^2$

Let's assume that the atoms are going to spend most of their time around their equilibrium positions, so we can try to keep the carbon as our reference point and introduce 3 displacement coordinates

$$q_1 = x_1 + l_0$$
$$q_2 = x_2$$
$$q_3 = x_3 - l_0$$

Just a shift of the location of the origin for each atom, l_0 is constant!

$$\frac{d}{dt} q_1 = \frac{d}{dt}(x_1 + l_0) = \frac{dx_1}{dt}$$

$$\frac{d^2 q_1}{dt^2} = \frac{d^2 x_1}{dt^2}$$

velocity & accelleration are the same!

$$V(q_1, q_2, q_3) = \frac{1}{2}k(q_2 - q_1)^2 + \frac{1}{2}k(q_3 - q_2)^2$$

Forces $= -\frac{\partial V}{\partial q}$

$$F_1 = -\frac{\partial V}{\partial q_1} = -\left[-k(q_2 - q_1)\right]$$
$$F_2 = -\frac{\partial V}{\partial q_2} = -\left[k(q_2 - q_1) - k(q_3 - q_2)\right]$$
$$F_3 = -\frac{\partial V}{\partial q_3} = -\left[k(q_3 - q_2)\right]$$

Equations of Motion: $F = ma$

$$m_O \frac{\partial^2 q_1}{\partial t^2} = k q_2 - k q_1$$

$$m_C \frac{\partial^2 q_2}{\partial t^2} = k\left[q_1 - 2q_2 + q_3\right]$$

$$m_O \frac{\partial^2 q_3}{\partial t^2} = k\left[q_2 - q_3\right]$$

We can divide all 3 equations by the mass:

$$\frac{d^2 q_1}{dt^2} = \frac{k}{m_0}\left[-q_1 + q_2\right]$$

$$\frac{d^2 q_2}{dt^2} = \frac{k}{m_c}\left[q_1 - 2q_2 + q_3\right]$$

$$\frac{d^2 q_3}{dt^2} = \frac{k}{m_0}\left[q_2 - q_3\right]$$

In Matrix Form:

$$d^2/dt^2 \begin{bmatrix} q_1 \\ q_2 \\ q_3 \end{bmatrix} = \frac{k}{m_0}\begin{pmatrix} -1 & 1 & 0 \\ \gamma & -2\gamma & \gamma \\ 0 & 1 & -1 \end{pmatrix}\begin{pmatrix} q_1 \\ q_2 \\ q_3 \end{pmatrix}$$

where

$$\gamma = \frac{m_0}{m_c}$$

If we have a vector $\vec{v}_1 = \begin{pmatrix} v_{11} \\ v_{12} \\ v_{13} \end{pmatrix}$ that is an eigenvector of this matrix:

$$\begin{pmatrix} -1 & 1 & 0 \\ \gamma & -2\gamma & \gamma \\ 0 & 1 & 1 \end{pmatrix}\begin{pmatrix} v_{11} \\ v_{12} \\ v_{13} \end{pmatrix} = \lambda_1 \begin{pmatrix} v_{11} \\ v_{12} \\ v_{13} \end{pmatrix}$$

eigenvalue

This would mean:

$$d^2/dt^2 \begin{pmatrix} v_{11} \\ v_{12} \\ v_{13} \end{pmatrix} = \frac{k}{m_0}\lambda_1 \begin{pmatrix} v_{11} \\ v_{12} \\ v_{13} \end{pmatrix}$$

And each of these vector elements would have a simple diff EQ: all constants

$$\frac{d^2 v_{11}}{dt^2} = \frac{k}{m_0}\lambda_1 \; v_{11}$$

$$v_{11}(t) = A\cos(\omega_1 t) + B\sin(\omega_1 t)$$

where $\omega_1 = \sqrt{\frac{k\,\lambda_1}{m_0}}$

One thing to note is that:

$$\begin{pmatrix} V_{11} \\ V_{12} \\ V_{13} \end{pmatrix} \longleftarrow$$

These all have the same solution! So this vector is a concerted motion of the 3 atoms moving together.

Let's solve these eigenvalues & eigen vectors:

$$\begin{vmatrix} -1-\lambda & 1 & 0 \\ \gamma & -2\gamma-\lambda & \gamma \\ 0 & 1 & -1-\lambda \end{vmatrix} = 0$$

$$-\lambda^3 - \lambda^2(2\gamma+2) - \lambda(2\gamma+1) = 0$$

$$\lambda\left[\lambda^2 + \lambda(2\gamma+2) + (2\gamma+1)\right] = 0$$

$$\lambda(\lambda+1)(\lambda+2\gamma+1) = 0$$

$$\lambda = 0 \qquad \lambda_2 = -1 \qquad \lambda_3 = -1-2\gamma$$

For the $\lambda_1 = 0$ eigenvalue, the eigenvector is easy:

$$\begin{pmatrix} -1 & 1 & 0 \\ \gamma & -2\gamma & \gamma \\ 0 & 1 & -1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = 0$$

$-a + b = 0 \longrightarrow a = b$

$\gamma(a - 2b + c) = 0$

$b - c = 0 \longrightarrow b = c$

$\therefore$ $a = b = c$, so the first eigenvector

$$\vec{V}_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}$$

For the $\lambda_2 = -1$ eigenvector:

$$\begin{pmatrix} 0 & 1 & 0 \\ \gamma & -2\gamma+1 & \gamma \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \begin{matrix} \rightarrow b = 0 \\ \rightarrow \gamma a + (1-2\gamma) b + \gamma c = 0 \\ \rightarrow b = 0 \end{matrix}$$

Using 2^{nd} line: $\gamma(a + c) = 0$

$a = -c$

$$\therefore \quad \vec{V}_2 = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$$

For the $\lambda_3 = -1-2\gamma$ vector:

$$\begin{pmatrix} 2\gamma & 1 & 0 \\ \gamma & 1 & \gamma \\ 0 & 1 & 2\gamma \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \qquad \begin{matrix} 2\gamma a + b = 0 \\ \gamma a + b + \gamma c = 0 \\ b + 2\gamma c = 0 \end{matrix}$$

$$a = \frac{-b}{2\gamma}, \quad c = \frac{-b}{2\gamma} = a$$

$$\vec{V}_3 = \begin{pmatrix} 1 \\ -2\gamma \\ 1 \end{pmatrix}$$

Now, what do these <u>mean</u>?

$\lambda_1 = 0$ $\qquad\qquad$ $\lambda_2 = -1$ $\qquad\qquad$ $\lambda_3 = -1-2\gamma$

$$\vec{V}_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \qquad \vec{V}_2 = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \qquad \vec{V}_3 = \begin{pmatrix} 1 \\ -2\gamma \\ 1 \end{pmatrix}$$

$$\omega_1 = \sqrt{\frac{-k}{m_0}\lambda_1} \qquad \omega_2 = \sqrt{\frac{-k}{m_0}\lambda_2} \qquad \omega_3 = \sqrt{\frac{-k}{m_0}\lambda_3}$$

$$\omega_1 = 0 \qquad \omega_2 = \sqrt{\frac{k}{m_0}} \qquad \omega_3 = \sqrt{\frac{k}{m_0}(1+2\gamma)}$$

Any constant times an eigenvector is still an eigenvector, even when that constant depends on time:

$$\vec{w}_1 = s_1(t)\begin{pmatrix}1\\1\\1\end{pmatrix}$$

$$\frac{d^2}{dt^2}\vec{w}_1 = \frac{k}{m_0}\begin{pmatrix}-1 & 1 & 0\\ \gamma & -2\gamma & \gamma\\ 0 & 1 & -1\end{pmatrix} s_1(t)\begin{pmatrix}1\\1\\1\end{pmatrix} = \frac{k}{m_0}s_1(t)\begin{pmatrix}-1 & 1 & 0\\ \gamma & -2\gamma & \gamma\\ 0 & 1 & -1\end{pmatrix}\begin{pmatrix}1\\1\\1\end{pmatrix}$$

$$= \frac{k}{m_0}s_1(t)\,\lambda_1\begin{pmatrix}1\\1\\1\end{pmatrix} = s_1(t)\begin{pmatrix}0\\0\\0\end{pmatrix}$$

Or:

$$d^2/dt^2\; s_1(t)\begin{pmatrix}1\\1\\1\end{pmatrix} = 0 \quad\Rightarrow\quad \frac{d^2}{dt^2}s_1(t) = 0$$

This tells us that when all 3 atoms move together in the same direction, the experience no accelleration. The molecule as a whole moves with constant velocity.

This mode: $\begin{pmatrix}1\\1\\1\end{pmatrix}$ is called a center-of-mass translation.

For Eigenvector 2:

$$\vec{w}_2 = s_2(t)\begin{pmatrix}1\\0\\-1\end{pmatrix}$$

$$\frac{d^2}{dt^2}\left[s_2(t)\begin{pmatrix}1\\0\\-1\end{pmatrix}\right] = \frac{k}{m_0}\begin{pmatrix}-1 & 1 & 0\\ \gamma & -2\gamma & \gamma\\ 0 & 1 & -1\end{pmatrix} s_2(t)\begin{pmatrix}1\\0\\-1\end{pmatrix}$$

$$\frac{d^2}{dt^2}\left[S_2(t)\begin{pmatrix}1\\0\\-1\end{pmatrix}\right] = \frac{k}{m_0} S_2(t)\, \lambda_2 \begin{pmatrix}1\\0\\-1\end{pmatrix}$$

$$= -\frac{k}{m_0} S_2(t) \begin{pmatrix}1\\0\\-1\end{pmatrix}$$

$$\therefore \quad \frac{d^2}{dt^2} S_2(t) = -\frac{k}{m_0} S_2(t)$$

$$S_2(t) = C_2 \sin(\omega_2 t + \phi_2) \qquad \omega_2 = \sqrt{\frac{k}{m_0}}$$

oscillatory solution — amplitude — frequency — phase

This motion:

1 0 -1

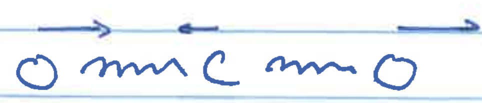
is called the symmetric stretch.

We get the same thing for $\vec{w}_3 = S_3(t)\begin{pmatrix}1\\-2\gamma\\1\end{pmatrix}$

with $S_3(t) = C_3 \sin(\omega_3 t + \phi_3)$

$$\omega_3 = \sqrt{\frac{k}{m_0}(1+2\gamma)}$$

This motion:



1 -2γ 1

is called the "asymmetric stretch"

In chemistry, these eigenvector motions are called normal modes, and the eigenvalues associated with them ~~that~~ tell us about vibrational frequencies.