So we have to solve the secular equation

$|A - \lambda I| = 0 \longleftarrow$ This is an n^{th} order polynomial so there will in general be n solutions

If A is Hermitian, these solutions $\lambda_i \quad i=1,\dots,n$ are real.

Why? A is Hermitian $\Longleftrightarrow A^\dagger = A^{*T} = A$.

$$A|r_j\rangle = \lambda_j |r_j\rangle$$

$\langle r_i|A|r_j\rangle = \lambda_j \langle r_i|r_j\rangle$. Taking the adjoint of this equation and noting that $\langle r_j| = |r_j\rangle^\dagger$

$$\langle r_j|A^\dagger|r_i\rangle = \lambda_j^* \langle r_j|r_i\rangle \Rightarrow$$

$$(\lambda_i - \lambda_j^*)\langle r_j|r_i\rangle = 0 \Rightarrow \lambda_i = \lambda_i^* \text{ and if } \lambda_i \neq \lambda_j$$

$\langle r_i|r_j\rangle = 0$. Of course, we know this from Q.M.

A couple of examples: $A = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$

The secular equation is:

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

$\lambda(\lambda^2 - 1) = 0$ so the roots are $\lambda = -1, 0, 1$

Let's find the eigenvector associated with $\lambda = -1$

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$$\begin{pmatrix} +1 & 1 & 0 \\ 1 & +1 & 0 \\ 0 & 0 & +1 \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \vec{0} \Rightarrow x+y=0 \text{ and } z=0$$

$|r_1\rangle = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}$ or, if we want to normalize it:

$$|r_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix} \qquad \lambda_1 = -1$$

for $\lambda = 0$ $\quad y=0,\ x=0 \Rightarrow |r_2\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix},\ \lambda_2 = 0$

for $\lambda = +1$ $\quad x-y=0,\ z=0 \Rightarrow |r_3\rangle = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}\frac{1}{\sqrt{2}},\ \lambda_3 = +1$

Note, these are all orthogonal to each other as we expect for a Hermitian matrix.

Another example – a matrix with degenerate eigenvalues:

$$A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix} \Rightarrow \text{secular equation } (1-\lambda)(\lambda^2-1) = 0$$

roots are $\lambda = -1, \underbrace{1, 1}$

Note: two degenerate roots.

for $\lambda = -1$ we can do the usual thing:

$$\lambda = -1 \Rightarrow 2x = 0 \quad +y+z=0 \Rightarrow |r_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}$$

Now for $\lambda = +1$ we have $x \cdot 0 = 0$ and

$-y+z=0$

So we have $|r_2\rangle = \begin{pmatrix} x \\ 1 \\ 1 \end{pmatrix}$ (Not normalized)

for any x.

We can choose $|r_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix}$, but how can we pick $|r_3\rangle$?

$$|r_3\rangle = \begin{pmatrix} x \\ 1 \\ 1 \end{pmatrix} + a\begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix} + b\begin{pmatrix} 0 \\ 1 \\ -1 \end{pmatrix}$$

want

$$0 = \langle r_1|r_3\rangle = a\cdot 0 + \frac{b\,2}{\sqrt{2}} \Rightarrow b = 0$$

$$0 = \langle r_2|r_3\rangle = \frac{1}{\sqrt{2}}\,2 + a\sqrt{2} = 0 \Rightarrow a = -1$$

$|r_3\rangle = \begin{pmatrix} x \\ 0 \\ 0 \end{pmatrix}$ ← take $x=1$. By the way, we used a process called Gram-Schmidt orthogonalization. We will discuss it more fully when we look at function spaces.

Working in a basis where A is diagonal. Note that we will assume here that A is Hermitian.
Note that $|r_i\rangle$ form a orthonormal basis. Any vector $|v\rangle$ can be expanded in this basis

$|v\rangle = a_i|r_i\rangle$ for some (complex) numbers a_i

In this basis, what is the matrix representation of A?

$$A \doteq |r_i\rangle\langle r_i|A|r_j\rangle\langle r_j|$$

So if we had a matrix representation of A in the $|\hat{e}_i\rangle$ basis where $|\hat{e}_1\rangle = |x\rangle$, $|\hat{e}_2\rangle = |y\rangle$, and $|\hat{e}_3\rangle = |z\rangle$ then

$$|\hat{e}_n\rangle\langle\hat{e}_n|A|\hat{e}_\ell\rangle\langle\hat{e}_\ell| = |r_i\rangle\langle r_i|e_n\rangle\langle e_n|A|e_\ell\rangle\langle e_\ell|r_j\rangle\cdot\langle r_j|$$

or

A in the original basis

$$A' = R^\dagger A R$$

A in the diagonal basis

where $R^\dagger_{in} = \langle r_i|e_n\rangle$

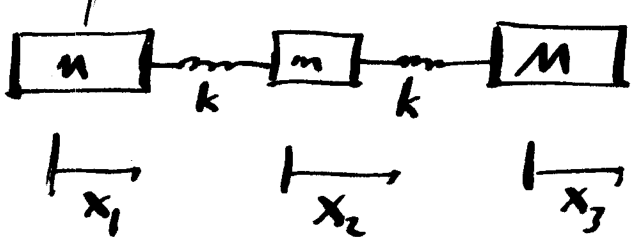
$R_{ni} = \langle e_n|r_i\rangle$

or

$$R = \begin{pmatrix} x_1 & x_2 & x_3 \\ y_1 & y_2 & y_3 \\ z_1 & z_2 & z_3 \end{pmatrix} \leftarrow \text{just columns of the eigenvectors.}$$

Notice that this is just a special case of a similarity transformation.

As an example, we can look at the normal modes of vibration of a molecule B–A–B.



$$M\ddot{x}_1 = -k(x_1 - x_2) \qquad M\ddot{x}_3 = -k(x_3 - x_2)$$

$$m\ddot{x}_2 = -k(x_2 - x_1) - k(x_2 - x_3)$$

Look for solutions of the form: $x_i = x_i^0 e^{i\omega t}$

$$\Rightarrow \quad -\omega^2 \begin{pmatrix} x_1^0 \\ x_2^0 \\ x_3^0 \end{pmatrix} = \begin{pmatrix} -k/M & k/M & 0 \\ +k/m & -2k/m & k/m \\ 0 & k/M & -k/M \end{pmatrix} \begin{pmatrix} x_1^0 \\ x_2^0 \\ x_3^0 \end{pmatrix}$$

To get nontrivial solutions we need:

$$\det \begin{pmatrix} k/M - \omega^2 & -k/M & 0 \\ -k/m & 2k/m - \omega^2 & -k/m \\ 0 & -k/M & \frac{k}{M} - \omega^2 \end{pmatrix} = 0$$

$$0 = \left(\frac{k}{M} - \omega^2\right)\left[\left(\frac{2k}{m} - \omega^2\right)\left(\frac{k}{M} - \omega^2\right) - \frac{k^2}{Mm}\right] + \frac{k}{M}\left[\frac{-k}{m}\right]\left[\frac{k}{M} - \omega^2\right]$$

$$-\omega^2 k/M$$

$$0 = \left[\frac{k}{M} - \omega^2\right]\left[\frac{2k^2}{mM} - \omega^2 \frac{2k}{m} + \omega^4 - \frac{k^2}{Mm} - \frac{k^2}{Mm}\right]$$

$$0 = \omega^2\left(\frac{k}{M} - \omega^2\right)\left(\omega^2 - \frac{2k}{m} - \frac{k}{M}\right)$$

There are three solutions for ω^2

$$\omega^2 = 0, \quad \omega^2 = k/M \quad \text{and} \quad \omega^2 = \frac{2k}{m} + \frac{k}{M}$$

We can now look at the eigenvector associated with these eigenvalues.

$\omega^2 = 0 \Rightarrow \quad x_1^\circ - x_2^\circ = 0$

$\qquad\qquad\quad -x_2^\circ + x_3^\circ = 0$

$\Rightarrow x_1^\circ = x_2^\circ = x_3^\circ$ Rigid body motion of the molecule.

Now try $\omega^2 = k/M \Rightarrow x_2^\circ = 0$ and from the middle equation: $x_1^\circ + x_3^\circ = 0 \Rightarrow$

For $\omega^2 = \frac{k}{M} + \frac{2k}{m} \Rightarrow -x_1^\circ \frac{2k}{m} - \frac{k}{M} x_2^\circ = 0$

$\Rightarrow x_2^\circ = -x_1^\circ \frac{2M}{m}$ and

$-\frac{k}{m}(x_1^\circ + x_3^\circ) - \frac{k}{M} x_2^\circ = 0$ or

$-x_1^\circ = \frac{m}{M} x_2^\circ + x_3^\circ \Rightarrow -x_1^\circ = -2x_1^\circ + x_3^\circ \Rightarrow$

$x_1^\circ = x_3^\circ$