Mathematics recap

— linear algebra continued —

Take a vector space, V. Operator

$$\hat{A} : V \to V$$

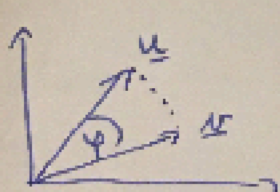
maps the vector space to itself. It means that for $\underline{v} \in V$

$$\hat{A}\,\underline{v} = \underline{u}$$

and $\underline{u} \in V$

Example for operators:

a) vectors in 2D space, $\hat{R}(\varphi)$: operator of rotation by angle φ



b) functions in $L^2(a,b)$ space, $\hat{D} = \frac{d}{dx}$ operator of differentiation

$$\hat{D}\,f = f'$$

The effect of operators can be ~~x~~ undone by the inverse:

$$\hat{A}^{-1}\hat{A} = \hat{E}$$

where $\hat{E}$ is the unit operator. That is for any $\underline{v} \in V$

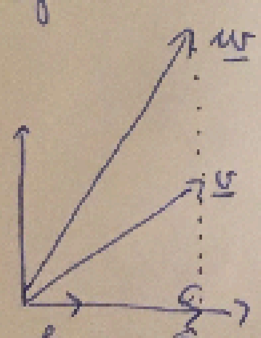
$$\hat{E}\underline{v} = \underline{v}$$

$$\text{and} \quad \hat{A}^{-1}\underline{u} = \underline{v} \quad \text{if} \quad \hat{A}\underline{v} = \underline{u}$$

HW: Find the inverse of $\hat{R}(\varphi)$ and $\hat{D}$ introduced ~~at~~ on page 21.
Be aware of the constant of integration, c.f. page 2

Important about operator inverse: not all operators can be inverted

Example: vectors in 2D space, $\hat{P}_1\underline{v} = \underline{e}_1 \langle \underline{e}_1 | \underline{v} \rangle$



$\hat{P}_1\underline{v} = \hat{P}_1\underline{w} = \underline{u}$

Since both $\underline{v}$ and $\underline{w}$ are mapped into $\underline{u}$ we will not find a $\hat{P}_1^{-1}$ that will map $\underline{u}$ once into $\underline{v}$, other time into $\underline{w}$.

Terminology: operators that do not have an inverse are called singular.

Note the analogy with division by zero. That is, the number $\emptyset$ does not have a multiplicative inverse. Note however, that $\hat{P}_1$ is <u>not</u> the Zero operator, that would give $\hat{\emptyset}\,\underline{v} = \emptyset$ for any $\underline{v}$.

Product of operators are understood as successive mappings. That is

$$\hat{B}\,\hat{A}\,\underline{v} = \hat{B}\,\underline{u}$$

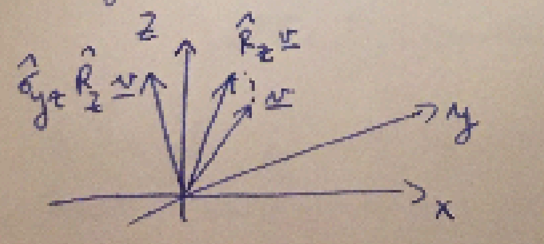
$$\uparrow$$

$$\hat{A}\underline{v} = \underline{u}$$

Example: vectors in 3D space

$\hat{R}_z(\varphi)$: rotation around axis z by angle φ, $\varphi < \pi/2$

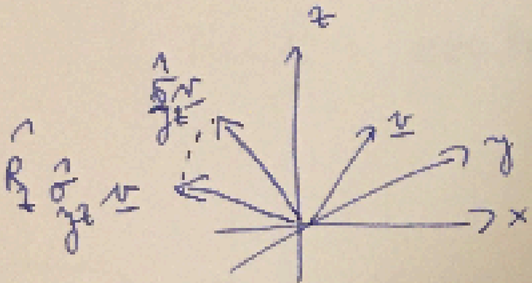
$\hat{\sigma}_{yz}$: reflection over plane yz



Starting from a $\underline{v}$ in plane xz, i.e.

$$\underline{v}\begin{pmatrix}\ast\\ \phi\\ \ast\end{pmatrix}\xrightarrow{\hat{R}_z}\begin{pmatrix}\ast\\ \ast\\ \ast\end{pmatrix}\xrightarrow{\hat{\sigma}_{yz}}\begin{pmatrix}-\ast\\ \ast\\ \ast\end{pmatrix}$$

Now let us investigate the reverse order operation



$$\underline{v}\begin{pmatrix}\ast\\ \phi\\ \ast\end{pmatrix}\xrightarrow{\hat{\sigma}_{yz}}\begin{pmatrix}-\ast\\ \phi\\ \ast\end{pmatrix}\xrightarrow{\hat{R}_z}\begin{pmatrix}-\ast\\ \ast\\ -\ast\end{pmatrix}$$

Obviously the result is different.

Important conclusion: order matters when multiplying operators!

In general

$$\hat{A}\hat{B} \neq \hat{B}\hat{A}$$

Terminology: $[\hat{A}, \hat{B}] = \hat{A}\hat{B} - \hat{B}\hat{A}$ is called a commutator

Further terminology: operators $\hat{A}$ and $\hat{B}$ are called commuting, when $[\hat{A}, \hat{B}] = \phi$.

Note: $[\hat{A}, \hat{B}] = \phi$ is not general and has some important consequences as we will see later.

{HW:} Take $L^2(a,b)$ space and show that $\hat{D} = \frac{d}{dx}$ and $\hat{A} = x\cdot$ do not commute.

The effect of $\hat{A}$: $\hat{A} f(x) = x \cdot f(x)$

Hint: evaluate $\hat{D}\hat{A} f(x)$ and $\hat{A}\hat{D} f(x)$ and compare.

{HW:} Take

$$f(x,y) = \ln\left(\frac{xy}{x+y}\right)$$

and show that $\hat{D}_x = \frac{\partial}{\partial x}$ and $\hat{D}_y = \frac{\partial}{\partial y}$ commute, by evaluating $\hat{D}_x \hat{D}_y f$ and $\hat{D}_y \hat{D}_x f$ and comparing.

Do you know by whom $\hat{D}_y \hat{D}_x = \hat{D}_x \hat{D}_y$ is named?

Important class of operators: linear operators.

A linear operator possesses two properties:

1) $\hat{A}(\gamma \underline{v}) = \gamma \hat{A} \underline{v}$ i.e. homogeneous

2) $\hat{A}(\underline{v} + \underline{w}) = (\hat{A}\underline{v}) + (\hat{A}\underline{w})$ i.e. additive

{HW:} Check that $\hat{R}(\varphi)$ and $\hat{D}$ given on page 21 are linear.

Note: nonlinear operators do occur in physics & chemistry but they count exotic. We will be concerned with linear operators only.

Example for a nonlinear operator:

$$\hat{A}\,\underline{v} = \frac{\langle \underline{v} | \underline{a} \rangle}{\langle \underline{v} | \underline{v} \rangle}$$ where $\underline{a}$ is a constant vector (nonzero)

HW: Prove, that $\hat{A}$ above is not linear.

Why are linear operators important? One reason is, that their effect is extremely easy to calculate on a vector given as a linear combination. We have been considering the form

$$\underline{w} = \sum_i \omega_i \underline{v}_i$$

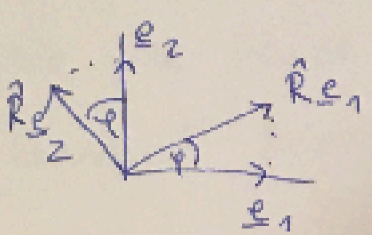
a lot in the first part, where $\{\underline{v}_i\}_{i=1}^{N}$ are ON basis vectors. Now evaluate $\hat{A}\,\underline{w}$:

$$\hat{A}\,\underline{w} = \hat{A} \sum_i \omega_i \underline{v}_i = \sum_i \hat{A}\, \omega_i \underline{v}_i = \sum_i \omega_i \hat{A}\,\underline{v}_i \quad (8)$$

↑ $\hat{A}$ is ~~linear~~ additive ↑ $\hat{A}$ is homogeneous

The importance of the result at the bottom of page 26 is: once we know the effect of $\hat{A}$ on the basis vectors we can calculate the effect of $\hat{A}$ on any vector.

Example: take $\underline{e}_1$ and $\underline{e}_2$ as ON basis vectors in 2D space



$$\hat{R}\underline{e}_1 = \cos(\varphi)\,\underline{e}_1 + \sin(\varphi)\,\underline{e}_2$$

$$\hat{R}\underline{e}_2 = -\sin(\varphi)\,\underline{e}_1 + \cos(\varphi)\,\underline{e}_2$$

can be inferred from the figure

$$\hat{R}\underline{e}_1 = \langle \underline{e}_1 | \hat{R}\underline{e}_1 \rangle \underline{e}_1 + \langle \underline{e}_2 | \hat{R}\underline{e}_1 \rangle \underline{e}_2$$

$$\hat{R}\underline{e}_2 = \langle \underline{e}_1 | \hat{R}\underline{e}_2 \rangle \underline{e}_1 + \langle \underline{e}_2 | \hat{R}\underline{e}_2 \rangle \underline{e}_2$$

We can even write this based on lecture 1.

Now assume $\underline{w} = \sum_{i=1}^{2} w_i \underline{e}_i$ and utilize (£) on page 26 to get

$$\hat{R}\underline{w} = \underline{e}_1 \left(\langle \underline{e}_1 | \hat{R}\underline{e}_1 \rangle w_1 + \langle \underline{e}_1 | \hat{R}\underline{e}_2 \rangle w_2 \right) +$$

$$+ \underline{e}_2 \left(\langle \underline{e}_2 | \hat{R}\underline{e}_1 \rangle w_1 + \langle \underline{e}_2 | \hat{R}\underline{e}_2 \rangle w_2 \right) \qquad (\$)$$

Arranging components of vector $\underline{w}$ into column vector

$$\underline{w}\begin{pmatrix} \omega_1 \\ \omega_2 \end{pmatrix} \qquad (@)$$

and introducing matrix $\underline{\underline{R}}$ as

$$\underline{\underline{R}}\begin{pmatrix} \langle \underline{e}_1 | \hat{R} \underline{e}_1 \rangle & \langle \underline{e}_1 | \hat{R} \underline{e}_2 \rangle \\ \langle \underline{e}_2 | \hat{R} \underline{e}_1 \rangle & \langle \underline{e}_2 | \hat{R} \underline{e}_2 \rangle \end{pmatrix} \qquad (\#)$$

we see that the matrix-vector product as learned from prof. István Szalai results

$$\underline{\underline{R}}\ \underline{w} = \begin{pmatrix} \langle \underline{e}_1 | \hat{R} \underline{e}_1 \rangle \omega_1 + \langle \underline{e}_1 | \hat{R} \underline{e}_2 \rangle \omega_2 \\ \langle \underline{e}_2 | \hat{R} \underline{e}_1 \rangle \omega_1 + \langle \underline{e}_2 | \hat{R} \underline{e}_2 \rangle \omega_2 \end{pmatrix}$$

that is just the vector in (\$) at the bottom of page 27, its components arranged ~~as~~ in a column. ~~vectors~~.

Note: for any operator the construction according to (#) above gives its

matrix representation.

The matrix representation of operators is the analogue of representing vectors with their components, c.f. (@) above.

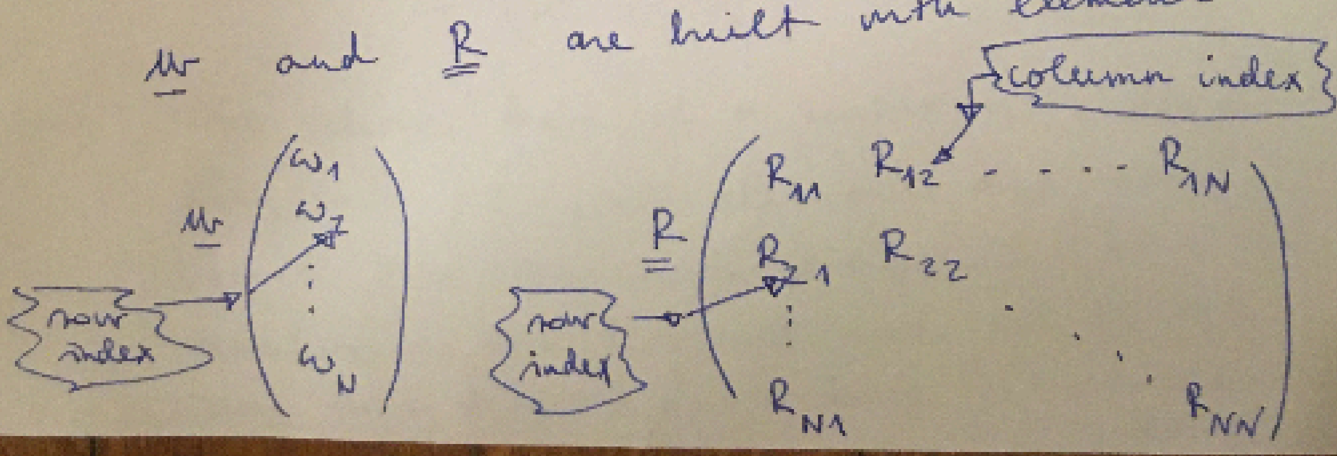
HW: Write the matrix representation of $\hat{\sigma}_{yz}$ in 3D space on Cartesian basis vectors $\underline{e}_x$, $\underline{e}_y$ and $\underline{e}_z$.

Hint: use (#) on page 28, that is determine $\hat{\sigma}_{yz}\underline{e}_x$, determine its expansion coefficients and fill the 3 components into the first column of $\underline{\underline{\sigma}}_{yz}$. Then proceed with $\hat{\sigma}_{yz}\underline{e}_y$ and fill the result into the second column of $\underline{\underline{\sigma}}_{yz}$. Finally $\hat{\sigma}_{yz}\underline{e}_z$ gives the third column.

HW: Write the matrix representation of $\hat{R}_z(\varphi)$ in the same manner.

Both are going to be used soon!

Remark: It is often convenient to write components of vectors and elements of matrices as indexed quantities. Hence $\underline{w}$ and $\underline{\underline{R}}$ are built with element



With indexed elements the matrix-vector product reads as

$$\left(\underline{\underline{R}}\,\underline{w}\right)_j = \sum_i R_{ji}\, w_i$$

note the column-row index matching

Let us get more abstract!

HW: Show that the elements of the unit operator $\hat{E}$ are δ_{ij}, where δ_{ij} is the Kronecker-delta symbol.

The unit operator leaves all vectors unchanged, i.e.

$$\hat{E}\,\underline{v} = \underline{v}$$

HW: Show, that the matrix corresponding to operator $\hat{A} = \lambda\cdot$ where λ is a number reads

$$\hat{A} \triangleq \begin{pmatrix} \lambda & & \emptyset \\ & \lambda & \\ \emptyset & & \ddots & \\ & & & \lambda \end{pmatrix} \qquad (\diamond)$$

Remark: The above form of a matrix is called diagonal, i.e. all elements are zero apart from the main diagonal. The numbers in the diagonal need not be the same for a diagonal matrix, hence $(\diamond)$ is even more special.

HW: Take the ON functions at the bottom of page 16, i.e. $v_1(x)$, $v_2(x)$ and $v_3(x)$ in $L_2(-1,1)$ space and construct the matrix representation of operator $\hat{D} = \frac{d}{dx}$ on this basis!

We step on by considering matrix products. Matrix products represent the product of operators. The recipe of matrix product evaluation in indexed form:

$$\left(\underline{\underline{A}}\,\underline{\underline{B}}\right)_{ij} = \sum_k A_{ik} B_{kj} \qquad (\approx)$$

note the column-row index matching

HW: Evaluate the product of matrices $\underline{\underline{\sigma}}_{yz}$ and $\underline{\underline{R}}_z$ calculated as instructed on page 29 in the order $\underline{\underline{\sigma}}_{yz}\underline{\underline{R}}_z$ and also $\underline{\underline{R}}_z\underline{\underline{\sigma}}_{yz}$ and verify that they are not the same. This way you have proven that $\hat{R}_z$ and $\hat{\sigma}_{yz}$ are non commuting, c.f. page 24.

{HW} Show that for any matrix $\underline{\underline{A}}$ and the unit matrix $\underline{\underline{E}}$, $[\underline{\underline{A}}, \underline{\underline{E}}] = \emptyset$ holds.

Hint: use $(\underline{\underline{E}})_{ij} = \delta_{ij}$ and evaluate $(\underline{\underline{E}}\,\underline{\underline{A}})_{ij}$ and $(\underline{\underline{A}}\,\underline{\underline{E}})_{ij}$ with the use of $(\approx)$ on page 31

We step on to discuss about operator inverse, in particular its matrix representation. For that we need the matrix transpose:

$$(\underline{\underline{A}}^T)_{ij} = (\underline{\underline{A}})_{ji}$$

i.e. matrix transpose arises by row - column swapping, and we also need the determinant, that we introduce via the example

$$\det\begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix} = A_{11}A_{22} - A_{21}A_{12}$$

{HW:} Show for the above matrix that

$$\det \underline{\underline{A}} = \det(\underline{\underline{A}}^T)$$

With the above we can construct the inverse of

$$\underline{\underline{A}} \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix}$$

as

$$\underline{\underline{A}}^{-1} = \frac{1}{\det \underline{\underline{A}}} \begin{pmatrix} A_{22} & -A_{12} \\ -A_{12} & A_{11} \end{pmatrix}$$

This is a 2x2 example. The general formula
of the inverse of $\underline{\underline{A}}$ involves its determinant
in the reciprocal and the so-called minors
of its transpose $\underline{\underline{A}}^T$. We need not go into
more detail on this.

HW: Check that $\underline{\underline{A}}\,\underline{\underline{A}}^{-1} = \underline{\underline{E}}$ indeed holds for
$\underline{\underline{A}}^{-1}$ above and $\underline{\underline{A}}$ at the bottom of page 22.

Important thing: we see now why the inverse
of an operator may be nonexisting. The
determinant of its matrix represantion must
be zero!

HW: Construct the matrix representation of
operator $\hat{P}_1$ at the bottom of page 22
on the basis $\{\underline{e}_i\}_{i=1}^{2}$ and verify that its
determinant is indeed zero.

Matrix inverse has an important field of
application, that is solving linear systems
of equations.

Example: suppose we have unknowns x_1 and x_2 fulfilling the equations

$$2x_1 + 3x_2 = 5$$
$$4x_1 + 5x_2 = 8 \qquad (*)$$

The matrix-vector form of the system of two equations above reads

$$\begin{pmatrix} 2 & 3 \\ 4 & 5 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 5 \\ 8 \end{pmatrix}$$

HW: ~~Prove, that~~ Calculate $\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 2 & 3 \\ 4 & 5 \end{pmatrix}^{-1} \begin{pmatrix} 5 \\ 8 \end{pmatrix}$ and

~~pro~~ substitute x_1 and x_2 into the equations above and see that they are fulfilled

Note: were $5x_2$ in $(*)$ above rather $6x_2$ the inverse would not be existing; in such case the linear system of equation has many solutions, c.f. example G18.10 on page 293

HW: Prove that $(\hat{A}\hat{B})^{-1} = \hat{B}^{-1}\hat{A}^{-1}$.

Some important things on operators appears in scalar products are due as the proceed

Consider vectors $\underline{u}$ and $\underline{v}$ and their transformation by ~~operator $\hat{U}$~~ matrix $\underline{\underline{U}}$, i.e.

$$(\underline{u}')_i = (\underline{\underline{U}}\,\underline{u})_i = \sum_j U_{ij} u_j$$

$$(\underline{v}')_i = (\underline{\underline{U}}\,\underline{v})_i = \sum_j U_{ij} v_j$$

Now consider the scalar product

$$\langle \underline{u}' | \underline{v}' \rangle = \sum_i u_i'^* v_i' = \sum_{\substack{i \\ jk}} (U_{ij} u_j)^* U_{ik} v_k =$$

$$= \sum_{jk} u_j^* \underbrace{\sum_i U_{ij}^* U_{ik}} v_k$$

if this was δ_{jk} then $\langle \underline{u}' | \underline{v}' \rangle = \langle \underline{u} | \underline{v} \rangle$ would hold

Hence when $\sum_i U_{ij}^* U_{ik} = \delta_{jk}$ holds then matrix $\underline{\underline{U}}$ does not change (i.e. conserves) the value of the scalar product. Such an ~~m~~matrix is called unitary.

The concise writing of the condition of unitary property is

$$\underline{\underline{U}}^{+} = \underline{\underline{U}}^{-1}$$

with the so-called adjoint matrix introduced

$$\underline{\underline{U}}^{+} = \left(\underline{\underline{U}}^{T}\right)^{*}$$ i.e. transposed and complex conjugated

{HW:} Write $\underline{\underline{U}}^{+}\underline{\underline{U}}$ with indices and show that indeed the expression at the bottom of page 35 results.

Important unitary operators are symmetry operators. E.g. rotation and reflection we used on page 23.

{HW:} Take the matrices of $\underline{\underline{\sigma}}_{yz}$ and $\underline{\underline{R}}_{z}$ constructed before and verify that they are unitary.

Another important property in connection with operators and scalar products is the self-adjoint or Hermitian property.

Matrix $\underline{\underline{H}}$ is self-adjoint if

$$\underline{\underline{H}}^{+} = \underline{\underline{H}} \quad .$$

When complex conjugation is irrelevant we speak of symmetric matrix, i.e. $\underline{\underline{H}}^{T} = \underline{\underline{H}}$. What does this have to do with scalar product?

Consider $\underline{u}$ and $\underline{v}$ and

$$\langle \underline{u} \,|\, \underline{\underline{H}}\,\underline{v} \rangle = \sum_i u_i^* \left(\underline{\underline{H}}\,\underline{v}\right)_i = \sum_{ij} u_i^* H_{ij} v_j$$

$$\langle \underline{\underline{H}}^{+}\underline{u} \,|\, \underline{v} \rangle = \sum_i \left(\underline{\underline{H}}^{+}\underline{u}\right)_i^* v_i = \sum_{ij} \underbrace{\left(H_{ji}^*\right)^*}_{H_{ji}} u_j^* v_i =$$

$$\underset{\substack{\uparrow \\ \text{summation indices can be swapped}}}{=} \sum_{ij} H_{ij} u_i^* v_j$$

hence we have $\langle \underline{u} \,|\, \underline{\underline{H}}\,\underline{v} \rangle = \langle \underline{\underline{H}}^{+}\underline{u} \,|\, \underline{v} \rangle$

HW: Take $L_2(-\infty, \infty)$ function space and $\hat{D} = \frac{d}{dx}$ and check ~~whether~~ whether $\hat{D}$ is Hermitian.

Hint: start from $\langle f \,|\, \hat{D} g \rangle = \int_{-\infty}^{\infty} f^*(x) \frac{d}{dx} g(x)\, dx$ and use integration by parts to get this in the form that can be related to $\langle \hat{D} f | g \rangle = \int_{-\infty}^{\infty} \left(\frac{d}{dx} f(x)\right)^{*} g(x)\, dx$.

Do they match? If not what makes the trouble?

We need to consider one more important thing about matrices and vectors, and that is a special type of equation called eigenvalue equation. The eigenvalue equation has the form

$$\underline{\underline{A}}\, \underline{v} = \lambda\, \underline{v} \qquad (\blacktriangledown)$$

~~where~~ $\underline{\underline{A}}$ ← known; $\underline{v}$, λ ← unknown

Terminology: $\underline{v}$: eigenvector

λ : eigenvalue

Special thing about the eigenvalue equation:

$\underline{\underline{A}}$ does not transform $\underline{v}$ into different orientation, it only alters its length. Such $\underline{v}$ are special from the point of view of $\underline{\underline{A}}$ and there are not many of them, if at least any.

Determining eigenvalues and eigenvectors of matrices:

$$(\underline{\underline{A}} - \lambda \underline{\underline{E}})\,\underline{v} = \underline{\emptyset}$$

rearranged form of (▼)

$(\underline{\underline{A}} - \lambda \underline{\underline{E}})$: nonzero matrix; $\underline{\emptyset}$: zero vector

The equation above can only hold if $(\underline{\underline{A}} - \lambda \underline{\underline{E}})^{-1}$ is not existing, i.e.

$$\det(\underline{\underline{A}} - \lambda \underline{\underline{E}}) = \emptyset$$

The above equation is called the secular equation and its solution gives the value of λ. There are ~~are~~ as many λ value as the dimension of the matrix, when $\underline{\underline{A}}$ is Hermitian. To each λ_i the ~~the~~ corresponding eigenvector v_i can be determined by substituting into the eigenvalue equation (▼) on page 38

HW: Find the eigenvalues of the matrix

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

Also find the corresponding eigvectors, that are normalized, i.e. $|\underline{v}_i| = 1$.

Note: the eigenvalue equation is homogeneous in $\underline{v}$, hence if $\underline{v}$ is a solution, so is $\gamma \underline{v}$ where γ is any nonzero number.

Eigenvalue equation written with indices:

$$(\underline{\underline{A}}\, \underline{v})_i = \lambda (v)_i$$

$$\sum_j A_{ij} v_j = \lambda v_i$$

Now introduce index 'k' referring to different solutions, this is the column index of $v_{..}$:

$$\sum_j A_{ij} v_{jk} = \lambda_k v_{ik} = \sum_j v_{ij} \delta_{jk} \lambda_k$$

Introduce also matrices

$$\underline{\underline{V}} \begin{pmatrix} v_{11} & v_{12} & \cdots \\ v_{21} & \ddots & \\ \vdots & & \end{pmatrix}$$

$$\underline{\underline{\lambda}}^{diag} \begin{pmatrix} \lambda_1 & & \\ & \lambda_2 & \emptyset \\ \emptyset & & \ddots \end{pmatrix}$$

That allows to write the matrix form of the eigenvalue equation as

$$\underline{\underline{A}}\, \underline{\underline{V}} = \underline{\underline{V}}\, \underline{\underline{\lambda}}^{diag}$$

Rearranging we get

$$\underline{\underline{V}}^{-1}\,\underline{\underline{A}}\,\underline{\underline{V}} = \underline{\underline{\lambda}}^{diag} \qquad (☺)$$

This construction is called a ~~simla~~ similarity transformation. (refers to $\underline{\underline{V}}^{-1}\,\underline{\underline{A}}\,\underline{\underline{V}}$)

This is called the diagonal form of matrix A (refers to $\underline{\underline{\lambda}}^{diag}$)

It can be shown that the similarity transformation performs a change of basis. The similarity transformation of (☺) is special because it is performed with the matrix built of the eigenvectors of $\underline{\underline{A}}$. It has the important property of getting $\underline{\underline{A}}$ into diagonal form.

The transformation of (☺) is also referred to as diagonalization. We will have to discuss some more about the eigen-problem of Hermitian matrices before closing this chapter in lecture 3.