Chem 623
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Review of Linear Algebra

Matrix – rectangular array of numbers

$$\begin{array}{cc} & \text{columns} \longrightarrow \\ A = \text{rows} \downarrow & \begin{bmatrix} 3 & 2 \\ 1 & 0 \\ 2 & 0 \end{bmatrix} \end{array}$$

3×2 matrix

\# of rows ↑ ↑ \# of columns

Operations

Matrix Addition

- only defined for matrices of the same size
- add term for term

Scalar Multiplication

- if K = constant and A = matrix
  KA obtained by multiplying each entry of A by K

$$3 \begin{bmatrix} 1 & 3 & 2 \\ 0 & -1 & 5 \end{bmatrix} = \begin{bmatrix} 3 & 9 & 6 \\ 0 & -3 & 15 \end{bmatrix}$$

Multiplication of Matrices

If A is an $m \times \underline{\underline{r}}$ matrix and if B is an $\underline{\underline{r}} \times n$ matrix, then the product

AB is an $m \times n$ matrix

order is <u>important</u>

Ex.

$$A = \begin{bmatrix} 1 & 1 & 5 \\ -1 & 0 & 2 \end{bmatrix} \qquad B = \begin{bmatrix} 0 & 8 & 1 \\ 2 & 8 & 2 \\ -1 & 3 & 1 \end{bmatrix} \qquad AB = \begin{bmatrix} -3 & 31 & 8 \\ -2 & -2 & 1 \end{bmatrix}$$

2x3 matrix   3x3 matrix   2x3 matrix

BA = undefined

Any linear system of equations can be expressed in terms of matrices

$$a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n = b_1$$
$$\vdots$$
$$a_{m1}x_1 + a_{m2}x_2 + \cdots + a_{mn}x_n = b_n$$

The above system is equivalent to:

$$AX = B$$

where

$$A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ \vdots & & & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix} \qquad X = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} \qquad B = \begin{bmatrix} b_1 \\ \vdots \\ b_m \end{bmatrix}$$

$m \times n$ matrix $n \times 1$ matrix $m \times 1$ matrix

$$\underbrace{AX}_{m \times 1 \text{ matrix}} = \underbrace{B}_{m \times 1 \text{ matrix}}$$

Trace

Defined only for square matrices
- sum of the elements on the main diagonal

$$A = \begin{bmatrix} 4 & 3 & 2 \\ 1 & 5 & 6 \\ 11 & 0 & -2 \end{bmatrix} \qquad tr(A) = 4 + 5 - 2 = 7$$

Transpose

If A is an $m \times n$ matrix, then A^t (A transpose) is an $n \times m$ matrix obtained by interchanging rows and columns of A.

Defined for all matrices!

$$A = \begin{bmatrix} 3 & -2 & 1 \\ 1 & 1 & -3 \end{bmatrix} \qquad A^t = \begin{bmatrix} 3 & 1 \\ -2 & 1 \\ 1 & -3 \end{bmatrix}$$

2×3 matrix

3×2 matrix

If A is a matrix with complex entries, then the <u>conjugate transpose</u> of A denoted by, A^*, is defined by

$$A^* = \bar{A}^t$$

where $\bar{A}$ is the matrix whose entries are the complex conjugates of the corresponding entries in A, and $\bar{A}^t$ is the transpose of $\bar{A}$

Ex. $A = \begin{bmatrix} 1+i & -i & 0 \\ 2 & 3-2i & i \end{bmatrix}$ $\bar{A} = \begin{bmatrix} 1-i & i & 0 \\ 2 & 3+2i & -i \end{bmatrix}$

$$A^* = \bar{A}^t = \begin{bmatrix} 1-i & 2 \\ i & 3+2i \\ 0 & -i \end{bmatrix}$$

Properties of transpose with A and B matrices with complex entries and k is any complex number

a) $(A^*)^* = A$
b) $(A+B)^* = A^* + B^*$
c) $(kA)^* = \bar{k} A^*$
d) $(AB)^* = B^* A^*$ ← order important

A square matrix A with complex entries is Hermitian if
$$A = A^*$$

Determinants

If A is a square matrix. The determinant of A, det(A) is define to be the sum of all signed elementary products from A.

The signed elementary products are obtained from the associated permutation so don't worry about the definition.

To obtain the determinant for a 2×2 matrix

$$\det \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} = a_{11}a_{22} - a_{12}a_{21}$$

For 3×3 case

$$\det \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = a_{11} \begin{vmatrix} a_{22} & a_{23} \\ a_{32} & a_{33} \end{vmatrix} - a_{12} \begin{vmatrix} a_{21} & a_{23} \\ a_{31} & a_{33} \end{vmatrix} + a_{13} \begin{vmatrix} a_{21} & a_{22} \\ a_{31} & a_{32} \end{vmatrix}$$

$$= a_{11}(a_{22}a_{33} - a_{23}a_{32}) - a_{12}(a_{21}a_{33} - a_{23}a_{31}) + a_{13}(a_{21}a_{32} - a_{22}a_{3}$$

<u>Thereom</u>: If A is any square matrix that contains a row of zeros, then $\det(A) = 0$

<u>Thereom</u>: A square matrix B has an inverse if and only if $\det(B) \neq C$

Vector space

<u>Subspace</u> - A subset W of a vector space V is a <u>subspace</u> of V if W itself is closed under addition and scalar multiplication.

Closed under addition means:

$$\text{If } \vec{u}, \vec{v} \in W \; , \; \vec{u} + \vec{v} \in W$$

$\in$: are contained in W

Closed under scalar multiplication means:

$$\text{If } \vec{u} \in W, \; k \in \mathbb{R} \text{ then } k\vec{u} \in W$$

<u>Def</u>: If $\vec{v}_1, \ldots, \vec{v}_r$ is a set in V such that every vector in V is a linear combination of $\vec{v}_1, \ldots, \vec{v}_r$, then we say that $\vec{v}_1, \ldots, \vec{v}_r$ <u>span</u> V ! For every $\vec{u} \in V$ there exists $k_1, \ldots, k_r$

$$\vec{u} = k_1\vec{v}_1 + k_2\vec{v}_2 + \cdots + k_r\vec{v}_r$$

<u>Def</u> $\{\vec{v}_1, \ldots, \vec{v}_r\}$ are <u>linearly independent</u> if

$$\vec{0} = k_1\vec{v}_1 + \cdots + k_r\vec{v}_r$$ has only the trivial solution (i.e. $k_1 = k_2 = \cdots = k_r = 0$ - only solution is zero, therefore this is a unique solution (only one possible))

$\{\vec{v}_1, \ldots, \vec{v}_r\}$ are linearly dependent if

$$\vec{0} = k_1\vec{v}_1 + \cdots + k_r\vec{v}_r$$ has nontrivial solutions

<u>Def</u> If V is any vector space and $S = \{v_1, v_2, \ldots, v_n\}$ is a set of vectors in V, then S is called a <u>basis</u> for V if the following two conditions hold :

(a) S is linearly independent
(b) S spans V

Eigenvalues, Eigenvectors

<u>Def</u>: If A is an $n \times n$ matrix, then a nonzero vector x in R^n is called an eigenvector of A if Ax is a scalar multiple of x; that is,

$$A\vec{x} = \lambda\vec{x}$$

for some scalar λ. The scalar λ is called an eigenvalue of A, and x is said to be an eigenvector of A corresponding to λ

$A\vec{x} = \lambda\vec{x}$ can also be written

$A\vec{x} = \lambda \cdot I\vec{x}$ where $I \equiv$ identity matrix

for 2×2

$$I = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

now $A\vec{x} - \lambda I\vec{x} = \vec{0}$

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

or

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

For existance of nontrival solutions

$$\det(\lambda I - A) = 0 \quad \text{or} \quad \det(A - \lambda I) = 0$$

Ex.

$$A = \begin{bmatrix} 2 & 0 \\ 1 & 5 \end{bmatrix}$$

$$\lambda I - A = \begin{bmatrix} \lambda - 2 & 0 \\ -1 & \lambda - 5 \end{bmatrix}$$

$$\det(\lambda I - A) = (\lambda-2)(\lambda-5) - (-1)(0) = 0$$

$\lambda_1 = 2 \quad \lambda_2 = 5$ eigenvalues

To find corresponding eigenvectors - substitute eigenvalues into $\lambda I - A$ and find basis for null space

<u>Def</u>: The <u>Nullspace</u> of A is the solution space of $A\vec{x} = \vec{0}$ in $\mathbb{R}^n$

For above example

$\lambda_1 = 2$

$$\begin{bmatrix} 2-2 & 0 \\ -1 & 2-5 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ -1 & -3 \end{bmatrix}$$

$-x_1 - 3x_2 = 0$

$x_1 = -3x_2$

let $x_2 = t$

$x_1 = -3t$

$$[x] = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = t \begin{bmatrix} -3 \\ 1 \end{bmatrix}$$

$$\text{let } \vec{v}_1 = \begin{bmatrix} -3 \\ 1 \end{bmatrix}$$

now, $\lambda_2 = 5$

$$\begin{bmatrix} 5-2 & 0 \\ -1 & 5-5 \end{bmatrix} = \begin{bmatrix} 3 & 0 \\ -1 & 0 \end{bmatrix} \xrightarrow[1^{st} + (3)\, 2^{nd}]{\text{row reduce}} \begin{bmatrix} 3 & 0 \\ 0 & 0 \end{bmatrix} \xrightarrow{(\frac{1}{3})\, 1^{st}} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}$$

$x_1 = 0$
$x_2 = t$

$$[x] = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = t \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$\text{let } \vec{v}_2 = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

now, $\vec{v}_1$ and $\vec{v}_2$ form a basis for nullspace

If k is a positive integer, λ is an eigenvalue of A, and $\vec{x}$ is a corresponding eigenvector, then λ^k is an eigenvalue of A^k and $\vec{x}$ is a corresponding eigenvector.

Example

$$A^2\vec{x} = A(A\vec{x}) = A(\lambda\vec{x}) = \lambda(A\vec{x}) = \lambda(\lambda\vec{x}) = \lambda^2\vec{x}$$

true for all k

Determining Eigenvectors

2/9/93

From Class

$$\begin{array}{cccc} |{++}\rangle & |{+-}\rangle & |{-+}\rangle & |{--}\rangle \\ \end{array}$$
$$\left[\begin{array}{c|cc|c} 2 & 0 & 0 & 0 \\ \hline 0 & 1 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ \hline 0 & 0 & 0 & 2 \end{array}\right]$$

Looking at the inner 2-by 2 matrix

$$A = \begin{array}{c} \begin{array}{cc} |{+-}\rangle & |{-+}\rangle \end{array} \\ \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \end{array}$$

Now, solve for eigenvalues as done previously

$$\det(\lambda I - A) = 0 \quad \text{or} \quad \det(A - \lambda I) = 0$$

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

$$(\lambda-1)(\lambda-1) - (-1)(-1) = 0$$
$$\lambda^2 - 2\lambda + 1 - 1 = 0$$
$$\lambda^2 - 2\lambda = 0$$
$$\lambda(\lambda - 2) = 0$$
$$\lambda = 0, 2 \quad \text{are eigen values}$$

Now, to get eigenvectors substitute eigenvalues back into matrix $(\lambda I - A)$ or $(A - \lambda I)$ and solve matrix

For $\lambda = 0$

$$\begin{bmatrix} 0-1 & -1 \\ -1 & 0-1 \end{bmatrix} = \begin{bmatrix} -1 & -1 \\ -1 & -1 \end{bmatrix} \xrightarrow[\text{1st} - \text{2nd}]{\text{row reduce}} \begin{bmatrix} -1 & -1 \\ 0 & 0 \end{bmatrix} \xrightarrow{(-1)\,\text{1st}} \begin{array}{c} \begin{array}{cc} |+-\rangle & |-+\rangle \end{array} \\ \begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix} \end{array}$$

now, the solution for the nullspace $A|\lambda=0\rangle = \vec{0}$ is

$$|+-\rangle + |-+\rangle = 0$$

$$|+-\rangle = -|-+\rangle$$

if we let $|-+\rangle = s$

then $|+-\rangle = -s$

where
* s is some arbitary value
* note: We are solving $|+-\rangle$ in terms of $|-+\rangle$. We could also do this the other way. This is just the arbitary phase.

Thus, the solution is

For $\lambda = 0$

$$|\lambda=0\rangle = \begin{bmatrix} |+-\rangle \\ |-+\rangle \end{bmatrix} = s \begin{bmatrix} -1 \\ 1 \end{bmatrix}$$

now, note that the value obtained is not normalized

$$\sqrt{(-1)^2 + (1)^2} = \sqrt{2} \neq 1$$

Therefore, divide by total length $\sqrt{2}$

$$|\lambda=0\rangle = \begin{bmatrix} |+-\rangle \\ |-+\rangle \end{bmatrix} = s \begin{bmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$$

let $\vec{v}_1 = \begin{bmatrix} -1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$

$$|\lambda=0\rangle = \frac{1}{\sqrt{2}}\left(-|+-\rangle + |-+\rangle\right) \quad \text{or} \quad \frac{1}{\sqrt{2}}\left(|+-\rangle - |-+\rangle\right)$$

phase difference between the two vectors

Similarly, for $\lambda = 2$

$$\begin{bmatrix} 2-1 & -1 \\ -1 & 2-1 \end{bmatrix} = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \xrightarrow{1^{st} + 2^{nd}} \begin{array}{cc} |+-\rangle & |-+\rangle \\ \end{array} \begin{bmatrix} 1 & -1 \\ 0 & 0 \end{bmatrix}$$

$$|+-\rangle = |-+\rangle$$

let $|-+\rangle = s$
$|+-\rangle = s$

$$|\lambda = 2\rangle = \begin{bmatrix} |+-\rangle \\ |-+\rangle \end{bmatrix} = s \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

normalizing

$$|\lambda = 2\rangle = s \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$$

let $\vec{V}_2 = \begin{bmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{bmatrix}$

$$|\lambda = 2\rangle = \frac{1}{\sqrt{2}} \left(|+-\rangle + |-+\rangle \right)$$

Now, lets show the original matrix $A = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}$ is orthogonally diagonalizable, We need to show that there exists an orthogonal matrix P such that $P^{-1}AP = D$ where D is a diagonal matrix whose entries are the eigenvalues of matrix A

From my previous Linear Algebra handout $\vec{V}_1$ and $\vec{V}_2$ form a basis for nullspace

Using $\vec{v}_1$ and $\vec{v}_2$ as column vectors (we already made them orthonormal) * note: the order of the column vectors is not important because the eigenvalue placement is arbitar

$$P = \begin{bmatrix} -1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix}$$

If $A = \begin{bmatrix} a & b \\ c & d \end{bmatrix}$ then

$$A^{-1} = \frac{1}{(ad-bc)} \begin{bmatrix} d & -b \\ -c & a \end{bmatrix}$$

then $$P^{-1} = \frac{1}{\left(-\frac{1}{2} - \frac{1}{2}\right)} \begin{bmatrix} 1/\sqrt{2} & -1/\sqrt{2} \\ -1/\sqrt{2} & -1/\sqrt{2} \end{bmatrix} = \begin{bmatrix} -1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix}$$

now $P^{-1} A P$

$$\underbrace{\begin{bmatrix} -1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}} \begin{bmatrix} -1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix}$$

$$\begin{bmatrix} 0 & 0 \\ 2/\sqrt{2} & 2/\sqrt{2} \end{bmatrix} \begin{bmatrix} -1/\sqrt{2} & 1/\sqrt{2} \\ 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 2 \end{bmatrix}$$

and $D = \begin{bmatrix} 0 & 0 \\ 0 & 2 \end{bmatrix}$ becouse $\lambda = 0, 2$ are eigenvalues of A

$\therefore$ A is orthogonally diagonalizable