Basic Course CPS615 Contact Points

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- CPS615 Powers that be above can be reached at cps615ad@npac.syr.edu
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- Homepage will be: http://www.npac.syr.edu/projects/cps615fall95

Course Structure

- Graded on the basis of Approximately 8 Homeworks, which will be due Wednesday of week following day given out (Monday or Wednesday)
- Plus one small project at the end of class
- No finals or written exams
- All material will be placed on World Wide Web (WWW)
- Preference given to work returned on the Web—optional lecture will be given on how to use WWW

Definition of a Matrix

- Consider matrix with elements A_{ij}
- It is an operator $\boldsymbol{A}$ in a vector space of dimension n where $\boldsymbol{A}$ is $n \times n$.
- There are n^2 numbers A_{ij} defining $\boldsymbol{A}$.
- The vector space is spanned by a "complete basis" $\underline{e}_k$, $k = 1 \ldots n$.
- One choice of $\underline{e}_k$ is

$$\begin{aligned} \underline{e}_1 &= (1, 0, 0, \ldots 0) \\ \underline{e}_2 &= (0, 1, \ldots 0) \\ \underline{e}_n &= (0, 0, \ldots 1) \end{aligned}$$

The Definition of a Vector

- Any vector $\underline{x} = (x_1, x_2, \ldots x_n)$ can be written in terms of the complete basis

$$\underline{x} = \sum_k x_k \underline{e}_k$$

- A_{ij} is representation of $\boldsymbol{A}$ in the basis $\{\underline{e}_k\}$
- The operator $\boldsymbol{A}$ operating on vector $\underline{x}$ is

$$\begin{aligned} \underline{y} &= A\underline{x} \\ \underline{y} &= \sum_l y_l \, \underline{e}_l \\ \underline{x} &= \sum_k x_k \, \underline{e}_k \\ \text{Components are } y_l &= \sum_k A_{lk} \, x_k \end{aligned}$$

- Physicists often write

$$\underline{x} = |x > \text{ called a ket}$$

The Definition of Scalar Products and Orthonormality

- $\underline{x}^T A \underline{x}$ is a number (scalar) written by physicists $\langle y|A|x\rangle$ where $\langle y|$ is called a Bra.
- The Bra-ket is $\langle y|x\rangle$ or scalar product
- Therefore,

$$\begin{aligned} A_{lk} &= \underline{e}_l^T \, A \, \underline{e}_k \\ &= \langle e_l|A|e_k\rangle \end{aligned}$$

  The components of A with respect to basis $\{\underline{e}_k\}$

- The basis $\{e_k\}$ is orthonormal

$$\begin{aligned} \langle \underline{e}_k|\underline{e}_l\rangle &= \delta_{lk} \\ &= 0 \qquad l \neq k \\ &= 1 \qquad l = k \end{aligned}$$

- $\delta_{lk} = 0$ unless $l = k$ when $\delta_{lk} = 1$ is Kronecker delta

Types of Matrices

- Useful Symbols
  $A^T =$ Transpose $\quad (A^T)_{ij} = A_{ji}$
  $A^* =$ Complex Conjugate $\quad (A^*)_{ij} = A^*_{ij}$
  $A^+ =$ Hermitean Conjugate $\quad (A^+)_{ij} = A^*_{ji}$
- $A = A^+$ Hermitean Matrix
- In physics, all nice matrices are hermitean—we can understand why when we study eigenvalues and eigenvectors.
- Hermitean operators have a complete set of eigenvectors with real eigenvalues.

Eigenvectors and Eigenvalues

- Suppose $A\underline{v} = \lambda\underline{v}$ ($\underline{v}$ is not all zeros), or $A|v>= \lambda|v>$, where $\underline{v}$ is an eigenvector of A with eigenvalue λ.
- Suppose $\underline{e}_1 = (1, 0, 0 \ldots 0)$ is an eigenvector of A with eigenvalue λ_1.

$$
\begin{aligned}
A\underline{e}_1 = \lambda_1\underline{e}_1 &= \sum_l (\lambda_1\delta_{l1})\,\underline{e}_l \\
\lambda_1\delta_{l1} &= \sum_k A_{l1}\delta_{k1} \\
A &= \begin{bmatrix} \lambda_1 & & \\ 0 & & \\ 0 & & \text{ANY} \\ 0 & & \text{VALUE} \\ 0 & & \\ \vdots & & \end{bmatrix}
\end{aligned}
$$

Structure of Matrix

- If A is also symmetric (Hermitean)

$$A = \begin{bmatrix} \lambda_1 & 0 & 0 & 0 & 0 & \ldots & 0 \\ 0 & & & & & & \\ 0 & & & & & & \\ 0 & & A & N & Y & & \\ 0 & & V & A & L & U & E \\ 0 & & & & & & \end{bmatrix}$$

- If $\underline{e}_2 \ldots \underline{e}_n$ are also eigenvectors with eigenvalues $\lambda_2 \ldots \lambda_n$,

$$\begin{aligned} \underline{e}_2 &= (0, 1, 0, \ldots 0) \\ \underline{e}_n &= (0, 0, \ldots 1) \end{aligned}$$

Then

$$A = \begin{bmatrix} \lambda_1 & & & & \\ & \lambda_2 & & 0 & \\ & & \lambda_3 & & \\ & 0 & & \ddots & \\ & & & & \lambda_n \end{bmatrix}$$

A is diagonal with diagonal entries λ_i.

Equations for Eigenvalues—I

- If $A\underline{v} = \lambda\underline{v}$
  $(A - \lambda I)\underline{v} = 0$
  - I is identity matrix
- $B = A - \lambda I$. Then we have

$$
\begin{array}{rcl}
B\underline{v} = 0 & \text{and} & \underline{v} \neq [0, \ldots 0] \\
b_{11}v_1 + b_{12}v_2 & \ldots & +b_{1n}v_n = 0 \\
\vdots & & \\
b_{n1}v_1 \ldots & \ldots & b_{nn}v_n = 0
\end{array}
$$

- n linear equations for n unknowns v_i. This will normally only have solution

$$v_1 = v_2 = \ldots = v_k = \ldots = v_n = 0$$

Equations for Eigenvalues—II

- Condition for nontrivial $\underline{v}$ to solve $B\underline{v} = 0$ is: determinant $(B) = 0$
- This corresponds to

$$
\begin{aligned}
&\bullet\ n = 2 \qquad \det B &=&\ b_{11}\, b_{22} - b_{12} b_{21} \\
&\bullet\ n = 3 \qquad \det B &=&\ b_{11} \det \begin{bmatrix} b_{22} & b_{23} \\ b_{32} & b_{33} \end{bmatrix} \\
&&-&\ b_{12} \det \begin{bmatrix} b_{21} & b_{23} \\ b_{31} & b_{33} \end{bmatrix} \\
&&+&\ b_{13} \det \begin{bmatrix} b_{22} & b_{23} \\ b_{32} & b_{33} \end{bmatrix}
\end{aligned}
$$

•and so on recursively

Polynomial Equations for Eigenvalues

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

$$\det \begin{bmatrix} a_{11}-\lambda & a_{12} & & \\ a_{21} & a_{22}-\lambda & & \\ & a_{32} & & \\ & & & \\ & & & a_{nn}-\lambda \end{bmatrix}$$

- so det $(A - \lambda I) = 0$ is a polynomial of degree n in λ. Coefficient of λ^n is $(-1)^n$, i.e., always nonzero.
- On general principles, we will ALWAYS have n solutions

$$\lambda = \lambda_1, \lambda_2, \ldots \lambda_n$$

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

General Properties of Eigenvalues

- The solutions are usually COMPLEX and in special cases degenerate
  - e.g., matrix $A = I$, the unit matrix has n degenerate eigenvalues $\lambda_k = 1$.
- Now consider special case when A is real and symmetric, or more generally, complex but hermitean when we will find eigenvalues are real.

Eigenvalues of Hermitean Matrices—I

- For Hermitean A, suppose

$$\begin{aligned} Av_k &= \lambda_k v_k \\ A_{ij} v_k)_j &= \lambda_k \, v_k)_i \end{aligned}$$

- Multiply both sides by $v_k)_i^*$ and sum over $i = 1 \ldots n$

-

$$\begin{aligned} \langle v_k | A | v_k \rangle &= \lambda_k \langle v_k | v_k \rangle \text{ or} \\ \sum_{i,j=1}^{n} v_k)_i^* \, A_{ij} \, v_k)_j &= \lambda_k \sum_i v_k)_i^* \, v_k)_i \end{aligned}$$

- Write this LHS $= \lambda_k$ RHS. The right hand side (RHS) is clearly real and nonzero

$$\begin{aligned} \text{RHS} &= \sum_i \left| v_k)_i \right|^2 \\ &= \langle v_k | v_k \rangle \end{aligned}$$

Eigenvalues of Hermitean Matrices—II

- On the other hand, complex conjugate equation,

$$\begin{aligned}
\text{LHS} &= \sum_{i,j=1}^{n} v_k)_i^* \, A_{ij} \, v_k)_j \\
\text{LHS}^* &= \sum_{i,j=1}^{n} v_k)_i \quad \underbrace{A_{ij}^*}_{\text{as hermitean } A_{i,j}^* = A_{ji}} \quad v_k)_j^* \\
&= \sum_{i,j=1}^{n} v_k)_i \, A_{ji} \, v_k)_j^*
\end{aligned}$$

- Now Interchange i and j labels

$$\text{LHS}^* = \sum_{i,j=1}^{n} v_k)_i^* \, A_{ij} \, v_k)_j = \text{LHS}$$

Therefore, LHS is real

- Formally, we can show this for

$$\begin{aligned}
\langle x|A|y\rangle^* &= \langle y|A^+|x\rangle \\
&= \langle y|A|x\rangle \text{if } A \text{ Hermitean}
\end{aligned}$$

- Taking $\langle x| = \langle y|$, we see $\langle x|A|x\rangle^* = \langle x|A|x\rangle$ if A Hermitean
- It follows that

$$\lambda_k = \frac{\Sigma_{i,j=1}^{n} \, v_k^*)_i \, A_{ij} \, v_k)_j}{\Sigma_{i=1}^{n} \, v_k^*)_i \, v_k)_i}$$

is ALWAYS real

Orthogonality of Eigenvectors of Hermitean Matrices

- Now take any two eigenvectors/values

$$
\begin{aligned}
A|v_1> &= \lambda_1|v_1> \\
A|v_2> &= \lambda_2|v_2> \\
\langle v_2|A|v_1\rangle &= \lambda_1\langle v_2|v_1\rangle \quad (\alpha) \\
\langle v_1|A|v_2\rangle &= \lambda_2\langle v_1|v_2\rangle
\end{aligned}
$$

- Take complex conjugate of this equation

$$
\begin{aligned}
\langle v_2|A^+|v_1\rangle &= \lambda_2^*\langle v_2|v_1\rangle \\
\langle v_2|A|v_1\rangle &= \lambda_2\langle v_2|v_1\rangle \quad (\beta) \\
\text{as } A = A^+ \qquad & \lambda_2 = \lambda_2^*
\end{aligned}
$$

- Subtract (α) and (β)

$$(\lambda_1 - \lambda_2)\langle v_2|v_1\rangle = 0$$

- either $\lambda_1 = \lambda_2$ or $\langle v_2|v_1\rangle = 0$ so eigenvectors of different eigenvalues are orthogonal.
- Note if $|v_1>$ and $|v_2>$ are distinct eigenvectors of same degenerate eigenvalue $\lambda_1 = \lambda_2$, then we can replace $|v_2>$ by $|v_2'>$ where $|v_2'>$ is a linear combination of $|v_1>$ and $|v_2>$, and $< v_1|v_2'>= 0$.

Orthonormal Eigenvectors and Unitary Transformation Matrices

- We choose to normalize each eigenvector

$$\langle v_k | v_k \rangle = \sum_{i=1}^{n} v_k^*)_i \, v_k \,)_i = 1$$

- and we have proved

$$\langle v_k | v_l \rangle = 0 \qquad l \neq k$$

- eigenvectors are ORTHOnormal whether or not eigenvalues are degenerate
- Define a matrix U so that columns of U^+ are orthonormal eigenvectors

$$U^+ = \begin{bmatrix} v_1)_1 & & v_n)_1 \\ v_1)_2 & & \\ v_1)_3 & & \\ & & \\ & & \\ v_1)_n & & v_n)_n \end{bmatrix}$$

- U is UNITARY $\qquad U^+U = I$
- This unitary condition is exactly the orthonormality condition.

Diagonal Form of General Hermitean Matrix—I

- Consider transformed matrix $\tilde{A}$ using U defined previously

$$\tilde{A} = U^* \begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & 0 & \\ 0 & & & \\ & & & \lambda_n \end{bmatrix} U$$

$$\uparrow$$

Diagonal

- By inspection

$$\tilde{A}|v_k >= \lambda_k |v_k >$$

i.e., $\tilde{A}$ and A give same result on each eigenvector.

Diagonal Form of General Hermitean Matrix—II

- But ANY vector

$$|x> = \sum_{k=1}^{n} x_k |v_k>$$

as $|v_k>$ must be complete as ORTHOnormal and n of them

- Then

$$\begin{aligned} \tilde{A}|x> &= \sum_{k=1}^{n} x_k \tilde{A}|v_k> \\ &= \sum_{k=1}^{n} x_k A|v_k> \\ &= A|x> \end{aligned}$$

and we have proven $\tilde{A} \equiv A$

- Thus,

$$A = U^{+} \text{ Diag.} \begin{bmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{bmatrix} U$$

Eigenvectors and Eigenvalues of Symmetric Matrices

- Above we have taken hermitean operator $A^+ = A$. If A real then $A^+ = A^T$ and $A^T = A$.
- Then eigenvectors can be taken to be real as equation $(A - \lambda_i I)|v_k>$ has real coefficients (we showed λ_k real).
- Then U is real

$$\begin{aligned} U^+ &= U^T \\ U^T U &= I \\ U &\text{ is ORTHOGONAL} \end{aligned}$$

Finite and Infinite Dimensional Matrices as Operators

- We have discussed matrices. These are "operators" in finite (n) dimensional linear space.
- You can generalize to infinite dimensional space.

  — e.g., space of "suitable" functions $f(x)$
- $\frac{d}{dx}$ is an operator!
- $\frac{d}{dx}f(x) = g(x)$ is another function.

  — e.g., another operator

$\frac{d}{dx}$ as an Operator and Its Scalar Products

- Consider the Integral

$$I = \int_a^b g(x) \frac{d}{dx} f(x) dx = \langle g|D|f\rangle$$

where D is operator $\frac{d}{dx}$.

- Integrate by parts.

$$\begin{aligned} I = & - \int_a^b f(x) \frac{d}{dx} g(x)\, dx \\ & + \left[f(x) g(x)\right]_a^b \end{aligned}$$

- The last term

$$\left[f(x) g(x)\right]_a^b = f(b)\, g(b) - f(a)\, g(a)$$

- We need to get rid of this surface (endpoint) term.

$i\frac{d}{dx}$ as a Hermitean Operator

- Suppose we consider periodic functions

$$
\begin{aligned}
f(b) &= f(a) \\
g(b) &= g(a)
\end{aligned}
$$

— i.e., impose particular boundary conditions

- Then surface term vanishes and

$$
\int_a^b g(x)\frac{d}{dx}f(x)\,dx = -\int_a^b f(x)\frac{d}{dx}g(x)\,dx
$$

- The operator $L = i\frac{d}{dx}$ with boundary conditions $f(a) = f(b)$ is Hermitean. The i in L cancels minus sign.
- Must include boundary conditions when discussing operators in infinite dimensional space

The Laplacian as a (Matrix) Operator

- $\nabla^2 = \frac{d^2}{dx^2} = -L\,L$
- $\left(\nabla^2\right)^\dagger = -L^\dagger L^\dagger = -L\,L = \nabla^2$
- Note: $(A\,B)^\dagger = B^\dagger A^\dagger$ in general
- Thus, ∇^2 ($\frac{d^2}{dx^2}$ in one dimension) is Hermitean (symmetric) operator

Mapping of Function Spaces to a Finite Number of Dimensions

- In solving differential equations numerically, we take infinite dimensional operators on space of functions and convert them to finite matrix operators in space of n dimensional vectors.
- The different numerical approaches correspond to different ways of mapping the infinite dimensional space to a finite space—there is no unique way and some are much better than others.