HW 5 Computational Physics

September 20, 2005 Due September 27

Do problems 1 through 4 by hand (except for plotting) and the rest using the computer

1. Consider the set of functions defined on $-1 \leq x \leq 1$ with periodic boundary conditions [i.e., $f(-1) = f(1)$].

   (a) Demonstrate, using the obvious rules for vector addition and scalar multiplication, that this set forms a vector space.

   (b) Show for this vector space that the rule
   $$\langle f|g\rangle = \int_{-1}^{1} f^*(x)g(x)\,dx$$
   is acceptable as the definition of an inner product.

   (c) Using this inner product show that the set of functions $e_n(x) = \frac{1}{\sqrt{2}}e^{in\pi x}$ with $n = 0, \pm 1, \pm 2, \ldots$ forms an orthornormal basis.

   (d) Some function $f(x)$ is expanded in the above basis,
   $$f(x) = \sum_{n=-\infty}^{\infty} f_n e_n(x),$$
   with coefficients $f_n = (-1)^n\sqrt{8}/(n\pi)^2$ when $n \neq 0$ and $f_n = \sqrt{2}/3$ when $n = 0$. Plot the real and imaginary parts of the function. Can you see what function it is? Snippet:

```
x = arange(-1.,1.+h,h)
fapprox = 0.*x
nmax = ...
for n in arange(-nmax,nmax+1):
      if n==0:
            fn = ...
      ...
      fapprox = fapprox + fn*exp(1.j*n*pi*x)/sqrt(2.)
fapproxreal = real(fapprox)
fapproximag = imag(fapprox)
```

   (e) Expand the function $f(x) = e^{3x}$ in the above orthornormal basis. That is, find the coefficients f_n in the expansion. Then plot the exact function and its expansion on the same graph to make sure your coefficients are correct.

2. Consider the set of functions defined on $0 \leq x \leq 1$ with boundary conditions $f(0) = f(1) = 0$.

   (a) Using the obvious rules for vector addition and scalar multiplication, show that this set forms a vector space.

(b) Show for this vector space that the rule

$$\langle f|g\rangle = \int_0^1 f^*(x)g(x)\,dx$$

is acceptable as the definition of an inner product.

(c) Using this inner product show that the set of functions $e_n(x) = \sqrt{2}\sin n\pi x$ with $n = 1, 2, 3, \ldots$ forms an orthonormal basis.

(d) Expand $f(x) = x(1-x)$ in this basis by finding the coefficients f_n in the expansion

$$f(x) = \sum_{n=1}^{\infty} f_n e_n(x).$$

Plot the exact function and its expansion on the same graph.

(e) When you work in a basis, formally any operator $\hat{\Omega}$ can be represented as a matrix with matrix elements

$$\Omega_{mn} = \langle e_m|\hat{\Omega}|e_n\rangle.$$

This is true (although not very useful) even for the basis given in (c) above. Calculate the matrix Ω representing the operator $\hat{\Omega} = \frac{d^2}{dx^2}$ in the basis (c).

3. Consider the set of functions defined on $0 \le x \le 1$ with boundary conditions $f(0) = f(1) = 3$. Using the obvious rules for vector addition and scalar multiplication, show whether or not this set forms a vector space.

4. Solve this problem by hand, not by computer. Consider the three vectors

$$|1\rangle = \frac{1}{\sqrt{6}}\begin{pmatrix} 1 \\ i \\ 2 \end{pmatrix}, \quad |2\rangle = \frac{1}{\sqrt{5}}\begin{pmatrix} 2 \\ 0 \\ -1 \end{pmatrix}, \quad |3\rangle = \frac{1}{\sqrt{30}}\begin{pmatrix} -1 \\ 5i \\ -2 \end{pmatrix}.$$

(a) Show that these form an orthonormal basis (i.e., evaluate $\langle i|j\rangle$ for $i, j = 1, 2, 3$).

(b) Calculate $\sum_{i=1}^{3}\langle i|i\rangle$.

(c) Calculate $\sum_{i=1}^{3}|i\rangle\langle i|$. (Here $\langle i|$ is the Hermitian conjugate of $|i\rangle$.)

5. Using the computer find the determinant and inverse of

$$A = \begin{pmatrix} 1 & 5 & 0 & 0 \\ 2 & 3 & 4 & 5 \\ 7 & 6 & 5 & 4 \\ 1 & 5 & 9 & 2 \end{pmatrix}.$$

Check to make sure that the inverse is correct by computing AA^{-1}. Snippet:

```
from LinearAlgebra import *
A = array( ((1,5,0,0), ...))  , Float)
print "A =\n",A
print "Determinant of A is",determinant(A)
B = inverse(A)
```

6. It is easy to find eigenstates numerically. Consider the matrix

$$H = \begin{pmatrix} 5 & 3 & 1 & 0 \\ 3 & 7 & 2 & 1 \\ 1 & 2 & 1 & 3 \\ 0 & 1 & 3 & 9 \end{pmatrix}.$$

   (a) Find the eigenvalues and eigenvectors of H numerically and print the result. Snippet: Again import `LinearAlgebra` and use

   ```
   evalues, evectors = eigenvectors(H)
   ```

   (b) Examine your results: multiply H into the first eigenvector and compare with the product of the first eigenvalue and the first eigenvector. Repeat this for each eigenvector/eigenvalue pair. Snippet:

   ```
   print matrixmultiply(H,evectors[0])
   print evalues[0]*evectors[0]
   ```

   (c) Put `V=transpose(evectors)` and calculate the matrix product `V`† $\cdot$ `H` $\cdot$ `V`. (The first transpose is needed because LinearAlgebra returns the eigenvectors as rows instead of columns.)

7. When you have a matrix with both large and small elements, you can get a good approximation to the eigenstates by setting the small elements to zero. Define $H = H_0 + V$ where

$$H_0 = \begin{pmatrix} 5 & 2 & 0 & 0 \\ 2 & 4 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 2 \end{pmatrix}, \qquad V = 0.01 \times \begin{pmatrix} 1 & 2 & 1 & 1 \\ 2 & 3 & 0 & 2 \\ 1 & 0 & 3 & 1 \\ 1 & 2 & 1 & 2 \end{pmatrix}.$$

Calculate the eigenvalues of H_0 and of H. How close are they to one another? Compare to the order of magnitude of the elements of V.

8. When a matrix is "block diagonal" the eigenstate problem breaks into smaller problems.

   (a) Find the eigenstates of

$$\begin{pmatrix} 1 & 3 & 0 & 0 \\ 3 & 4 & 0 & 0 \\ 0 & 0 & 5 & 3 \\ 0 & 0 & 3 & 8 \end{pmatrix}.$$

   (b) Now find the eigenstates of

$$\begin{pmatrix} 1 & 3 \\ 3 & 4 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 5 & 3 \\ 3 & 8 \end{pmatrix}.$$

   You should get the same result as (a). Explain how to relate the 2D eigenvectors here with the 4D eigenvectors in (a).

Vector Spaces

A **linear vector space** $\mathbb{V}$ is a set of objects (the vectors) along with definite rules for vector addition and scalar multiplication which satisfy the following rules. (Here the vectors are denoted by lower-case Roman letters $\mathrm{a}, \mathrm{b}, \mathrm{c}, \ldots$ and scalars by lower-case Greek letters $\alpha, \beta, \ldots$.)

(a) **Vector addition**, denoted $\mathrm{a}+\mathrm{b}$, must satisfy the following:

  i. Closure: $\mathrm{a}+\mathrm{b} \in \mathbb{V}$
  ii. Commutivity: $\mathrm{a}+\mathrm{b}=\mathrm{b}+\mathrm{a}$
  iii. Associativity: $(\mathrm{a}+\mathrm{b})+\mathrm{c}=\mathrm{a}+(\mathrm{b}+\mathrm{c})$
  iv. Identity: there exists a null vector $\varnothing$ for which $\mathrm{a}+\varnothing=\mathrm{a}$ for all a
  v. For every vector a there exists an additive inverse, denoted $-\mathrm{a}$, for which $\mathrm{a}+(-\mathrm{a})=\varnothing$

(b) **Scalar multiplication**, denoted $\alpha\mathrm{a}$, must satisfy the following:

  i. Closure: $\alpha\mathrm{a} \in \mathbb{V}$
  ii. Associativity: $\alpha(\beta\mathrm{c})=(\alpha\beta)\mathrm{c}$
  iii. Distributivity in vectors: $\alpha(\mathrm{a}+\mathrm{b})=\alpha\mathrm{a}+\alpha\mathrm{b}$
  iv. Distributivity in scalars: $(\alpha+\beta)\mathrm{a}=\alpha\mathrm{a}+\beta\mathrm{a}$
  v. Identity: $1\mathrm{a}=\mathrm{a}$

Inner Product Spaces

Inner products can be denoted (a, b) or $\mathrm{a} \cdot \mathrm{b}$ or (my preference) $\langle\mathrm{a}|\mathrm{b}\rangle$.

An **inner product** $\langle\mathrm{a}|\mathrm{b}\rangle$ of two vectors is a definite rule that produces a scalar and satisfies:

$$\begin{aligned} \langle\mathrm{a}|\mathrm{b}\rangle &= \langle\mathrm{b}|\mathrm{a}\rangle^{*} \\ \langle\mathrm{a}|\beta\mathrm{b}+\gamma\mathrm{c}\rangle &= \beta\langle\mathrm{a}|\mathrm{b}\rangle+\gamma\langle\mathrm{a}|\mathrm{c}\rangle \end{aligned}$$

The only useful inner products in Physics are also positive semi-definite, which means:

$$\langle\mathrm{a}|\mathrm{a}\rangle \geq 0, \quad \text{and} \quad \langle\mathrm{a}|\mathrm{a}\rangle=0 \quad \text{iff} \quad \mathrm{a}=\varnothing .$$