Matlab Instruction Primer; Chem 691, Spring 2016

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CONTENTS

I. HELP: TO OBTAIN INFORMATION ABOUT ANY INSTRUCTION IN MATLAB

```
help 'instruction'    % 'instruction' can be any command
```

or hit ? on the matlab menu bar. Then go to `MATLAB/Getting Started`

or go to the MATLAB Academy.

II. SCRIPTING

Example: $f = A\cos(\omega t)$

```
A=30;           % specify parameters, semicolon silences the return
                     %percentage sign allows comment to follow
ome=2.5;             % you specify the variable name
t=0.1;
f=A*cos(ome*t)       % built-in function 'cos(x)'. no semicolon so the result is printed out
A=30;ome=2.5;t=0.1;f=A*cos(ome*t) % one line equivalent
```

Problem 1

The wavefunction for the ground state of the harmonic oscillator with reduced mass μ and force constant k is

$$\psi_0(x) = \left(\frac{\alpha}{\pi}\right)^{1/4} e^{-\alpha x^2/2}$$

where $\alpha = \sqrt{k\mu}$. For the H_2 molecule $\mu = 918$ (atomic units) and $\omega = 0.02$ (atomic units). Calculate k and α given that $\omega = \sqrt{k/\mu}$. The value of r_e for H_2 is 1.4 bohr (atomic units).

Defining $x = r - r_e$ write (and save) a Matlab script to determine $\psi_0(r = 1.5)$.

III. LOOPS, DETERMINE AN ARRAY OF VALUES, PLOT THE RESULT

```
for it = 1:100       % 'it' is counter, following fortran convention names of integers start
                     % with i,j,k,l,m,n but this is not necessary
   t = 0.05*it;      % determine successive time intervals; note looped commands are indented
   f(it)=A*cos(ome*t); % store result as a vector f
end                  % terminate loop

size(f)              % check size of the vector (it should be 100 x 1 (100 rows 1 column)

% plot result

 plot(f)             % just plot result, with integer abscissa
 plot(0.05*[1:100],f,'linewidth',1)          % plot result f vs t
                     %change width of line from 0.5 px (default) to 1
 xlabel('time / s')  % label x axis
 ylabel('function') % label y axis
```

```
set(gca,'fontsize',14) % increase size of lables

help plot           % find out about the many plotting options
```

Problem 2

Write a loop to determine the H_2 v=0 vibrational wavefunction at r=[0.8:0.02:1.9]. Call this array `psi_values`. Then plot these points.

IV. WORK WITH FUNCTIONS SYMBOLICALLY

```
clear A t ome        % clear values of variables
clear all            % clear all variables from workspace

syms A t ome         % declare A, T, omega as symbolic variables
f=A*cos(ome*t)       % redefine f in terms of symbolic variables
diff(f,t)            % derivative of f with respect to t
diff(f,A)            % derivative of f with respect to A
int(f,t)             % indefinite integral
int(f,t,pi/4,2*pi)      % definite integral

subs(int(f,t,pi/4,2*pi),[A ome],[30 1.2]) % give a definite value to omega
                                          % in the result of the integration

single(ans)            % numerical value for answer

g=exp(A*t)/(1+t^2)     % more complicated expression
pretty(g)              % display the expression for f more clearly

ff=subs(f,[A ome],[30 2.5]) % give definite values to two of the parameters in f(A,ome,t)

ezplot(ff,[-2 4])      % plot the result for -2 <= t <= 4
```

Problem 3

Declare the symbolic variables α and x, then define $\psi_0(x,\alpha)$ as a symbolic function `psi0`. *NB* The symbolic variable α should be defined as positive, namely

```
syms alpha x
assume(alpha,'positive') % note the apostrophes
```

Show that $\psi_0(x)$ is normalized

```
int(psi0*psi0,-inf,inf)
```

The wavefunction for v=2 is

$$\psi_2 = \left(\frac{\alpha}{\pi}\right)^{1/4} \frac{1}{\sqrt{2}}(2\alpha x^2 - 1)e^{-\alpha x^2/2}$$

Define a symbolic function `psi2` for $\psi_2(x)$ and show that $\langle 2|2\rangle = 1$ and $\langle 2|0\rangle = 0$

The harmonic oscillator Hamiltonian is $\hat{H}(x) = \hat{T} + \hat{V} = -\frac{1}{2\mu}\frac{d^2}{dx^2} + \frac{1}{2}kx^2$. Use your symbolic expression for $\psi_0(x)$ to show that

$$\langle 0|\hat{V}|0\rangle = \omega/4$$

and

$$\langle 0|\hat{T}|0\rangle = \omega/4$$

Hint Remember that $\alpha = \sqrt{k\mu} = \omega\mu$.

V. FUNCTIONS

A. Anonymous functions

```
g=@(t)30*cos(2.5*t)     %the '@(t)' denotes a function of the variable t
ezplot(g,-2,4)          %use ezplot to plot the function

fminbnd(g,1,2)          % find the minimum of g in the range 1 <= t <= 2

gg=matlabFunction(ff)    % convert any symbolic expression ff to a function
                         % note upper case F

int(ff,0,pi)             % integrate ff from 0 to pi

integral(gg,0,pi)        % numerically integrate the anonymous function from 0 to pi
```

VI. MINIMUM OF DISCRETE DATA

```
tt=[1 1.2 1.4 1.6 1.8] % five values of t
gx=g(tt) % 30 cos(2.5 t) at these five values
plot(tt,gx,'o-') % plot the four values, note the 'o-' commands a line-point plot

cc=polyfit(tt,gx,3)    % fit these points with a cubic polynomial

rr=roots(polyder(cc))     % find the roots of the derivative of cc, this defines the minima
                       % note that only one value [rr(2)] lies in the range 1 < t < 1.8
polyval(cc,rr(2))      % determine the value of the function at this value
```

Problem 4

As a further example you can define an anonymous function of two variables for the wavefunction of the harmonic oscillator

```
ppsi0=@(alpha,xx)(alpha/pi)^(1/4)*exp(-alpha*xx.*xx/2)
  % note that i'm using a different name for the independent
  % variable and for the function, so as not to redefine the symbolic variables psi0 and x
  % also note that i'm making the definition so that the variable can be a vector in which case
  % use '.*' invoking element-by-element multiplication (see the Linear Algebra section below).
```

Then you can define a vector of independent variables, and obtain at once the values of $\psi_0(x)$,

```
t=[0:0.01:1];
plot(t,ppsi0(20,t)) % no FOR loop needed.
  % Also, the name of the independent variable doesn't have to be xx
```

Define, similarly, an anonymous function of two variables (α and x) for the v=2 wavefunction. Call this function `psi2(alpha,xx)`. Obtain a vector of values of `psi2`, and plot. Using the Matlab function `ginput(1)`, obtain an estimate of the root of this function. Then, fit 4 points (call these `xxx`) around the root.

```
xxx=[0 .1 .2 .3] % guess that these straddle the root
cc=polyfit(xxx,psi2(alpha,xxx),3);
rr=roots(cc)    %  there will be several roots, pick the one that's physically reasonable
% this should be close to the value you got by graphical interpolation
```

VII. LINEAR ALGEBRA

```
vec=[.1 .2 .4 ]       % define a row vector of 3 elements
vec'                   % the prime is the transpose, converting this to a column vector

vec*vec'               % the dot product

vec'*vec               % the outer product


mat=[.1 .2 .3; .4 .2 -.3;.5 1 0] % a 3x3 matrix, the semicolon indicates the end of a line

mat(:,1)               % outputs the first column of the matrix as a column vector

mat(2,:)               % outputs the 2nd row of the matrix as a row vector

mat*vec                % a matrix-vector product (the result is a column vector)

mati=inv(mat)          % the inverse of a matrix

mati*mat               % the product of mat times its inverse; this is equal to the unit matrix

identity(3)            % the 3x3 unit matrix

mats=mat+mat'           % create a symmetric matrix


eig(mats)               % the eigenvalues of this matrix

[evec eval]=eig(mat)           % eigenvectors and eigenvalues of mats

diag([.1 .2 .3 .4])     % create a diagonal matrix with [.1 .2 .3 .4] along the diagonal
```

Matlab has an important property, that allows element-by-element multiplication or division of two vectors (or matrices) of the same size

```
vecm=vec.*vec; (or vecd=vec./vec;) % note the '.' which precedes the
   % multiplication or division
```

Problem 5

Define the symbolic variables `cs`, `sn`, `H11`, `H12` and `H22`. where $cs \equiv \cos(\theta)$ and $sn \equiv \sin(\theta)$ Define the matrices

```
C=[cs sn;-sn cs]

H=[H11 H12;H12 H22]

E = C.'*H*C           % diagonalize H
E = simplify(E)      % simplify E
```

Then, determine the value of θ so that the off-diagonal matrix element of the `C` matrix vanishes. With this value of θ, determine the values of the diagonal matrix elements E_{11} and E_{22}.

Note: Here, use the symbolic capability of Matlab to help you solve the problem. You'll have to do some simple algebra on your own at the end, to finish the problem.