Programs and functions

While using MATLAB as a fancy calculator has its own uses. It is also possible to use MATLAB as a programming language and to develop with it significant codes with considerable ease.

Files that end with .m are recognized as MATLAB program (or functions) and can be executed in MATLAB by typing their name. For example, the text below is kept in a file plotlog.m

```
% plot log(x) versus x
x = linspace(1,10);
y = log(x);
plot(x,y)
```

The first line is a comment in the file that tells us what the program is all about (it is plotting the log function) In the first line we assign to the array x 100 points between 1 and 10. The second line compute the log(x) (natural logarithm) and the third line plots x versus y.

To execute this program all we need to do is to type the name of the file (plotlog) in MATLAB main console and the complete file will be executed.

Note that the directory in which the *.m file is in must be included in the list of directories that MATLAB search for such a program. Choose from “File” the “set path” option to add a directory to the current list.

Of course the program as described do not receive input in a direct way (it is possible to initialize the relevant variables (if any) with the same name just before calling the .m file, however, this requires knowing more on the file that we want. The method below, using functions, is much better.

MATLAB allows the use of functions. Similarly to the program mentioned above they are always stored in .m files. The name of the function as called from the main window of MATLAB must be the same as the name of the file.

Consider an example of a function to compute the volume of a sphere, given the sphere radius

The syntax of the first line in a function is:

function [output] **= function_name**(input parameters)

```
function [volume] = volsph(r)
% volsph - a function to compute the volume of a sphere
% r is the radius (input), "volume" the volume (output)
% THE COMMENTS  THAT COME IMMEDIATELY
%  AFTER THE “function …” LINE
% ARE PRINTED WHEN TYPING “help function_name”
%

volume = (4.*pi/3.)*(r.^3);
```

The name of the file is volsph.m

Here is an example of a use of the function in the main window of MATLAB:

```
>> volsph(5)

ans =

  523.5988
```

Or, computing in one call couples of volumes

```
>> r = [1,2,3,4,5];
>> vol = volsph(r);
>> vol

vol =

    4.1888   33.5103  113.0973  268.0826  523.5988
```

Input and output

Here is an example of getting input directly from the main window:

```
>> a = input(' type in something \n ')
 type in something
 1

a =

     1
```

The command a " a= input(' type in something \n ') " echoes to the screen the expression enclosed within the quotes '…' the "\n" means opening a new line. Whatever is typed as a response is placed as the value of the "a".

Of course, for getting in a lot of data we need to be able to read from a file. Here is a quick introduction to fscan

The text below is a part of a file (name 1bii.ca) that includes a series of points (x,y,z coordinates).

```
       19.842  31.925  54.112
       19.411  33.862  50.859
       16.466  35.443  48.997
       15.760  36.986  45.649
       13.746  39.450  43.589
       13.651  38.210  39.954
       11.896  39.631  36.876
       10.937  37.345  33.994
       10.155  39.213  30.789
        8.895  37.761  27.498
        8.413  39.265  24.006
        7.029  37.077  21.245
        6.677  38.387  17.687
        3.525  37.515  15.771
        3.652  38.703  12.134
        0.328  36.961  11.420
       -1.414  38.234  14.565
       -0.102  41.838  15.052
        2.488  43.625  17.254
        4.463  41.562  19.795
        2.880  40.154  22.875
        4.916  41.493  25.783
        4.818  40.384  29.440
        6.616  41.042  32.712
        6.452  38.720  35.712
        7.948  39.620  39.140
        8.937  37.066  41.830
       10.219  37.016  45.410
       11.626  33.484  45.836
        9.088  30.957  44.396
        6.279  33.493  44.791
.
.
.
```

We want to read all the points into three arrays (x, y, and z with the Cartesian coordinates) without knowing in advance the length of the file. This is (relatively) simply done with fscanf and fopen. Below is a small function to do that preceded by the calling Line from the main window

MATLAB console

```
[x1,y1,z1] = get_points('1bii.ca');   % get the Cartesian coordinates from 1bii.ca into x1,y1,z1
```

And the function…

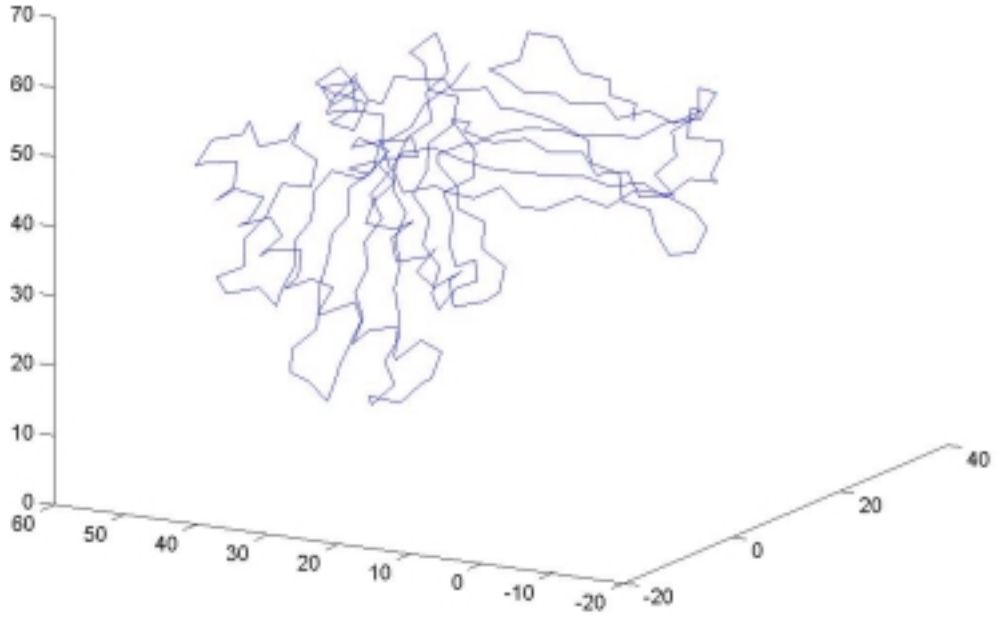
```
function [x,y,z] = get_points(filename)
% read set of points from a file (each line x,y,z coordinates)
% and return the results in 3 arrays x,y, and z
%

fid = fopen(filename);
crd = fscanf(fid,'%f');
dim = length(crd);
x = crd(1:3:dim-2);
y = crd(2:3:dim-1);
z = crd(3:3:dim);
```

Note that fscanf is reading to the end of the file (unless being instructed otherwise, see help fscanf for more details). The coordinates are read as one very long vector in which the x, y, and z coordinates are stored as x1,y1,z2,x2,y2,z2,… By manipulation of the indices we create the three desired arrays.

The points present a shape of a protein. The protein is a one-dimensional chain and each point corresponds to the CA of an amino acid. Connecting them by a curve as embedded in 3D is done by the simple command (in the console of MATLAB):

```
plot3(x1,y1,z1)
```

Can you identify secondary structure elements?


70
60
50
40
30
20
10
0
60
50
40
30
20
10
0
-10
-20
-20
0
20
40

Plotting protein structures:

The protein data bank is at www.rcsb.org (Research Collaboratory for Structural Bioinformatics). A gentle introduction to protein structures can be found in:
Carl Branden & John Tooze, "Introduction to Protein Structure", Garland Publishing NY 1991

PDB files are formatted and include more information that we need or want during this class.

The files open with comments, references and classifications of experimental techniques and structural features. We will be interested in the coordinates. These are lines that start with the keyword ATOM.

Here are typical ATOM entries:

```
ATOM      1  N   VAL     1      -4.095  14.896  13.982  1.00 17.14      1MBC  88
ATOM      2  CA  VAL     1      -3.483  15.451  15.217  1.00 17.16      1MBC  89
ATOM      3  C   VAL     1      -2.562  14.402  15.817  1.00 15.95      1MBC  90
ATOM      4  O   VAL     1      -2.966  13.230  15.884  1.00 17.17      1MBC  91
ATOM      5  CB  VAL     1      -4.592  15.944  16.184  1.00 18.07      1MBC  92
ATOM      6  CG1 VAL     1      -4.213  17.270  16.885  1.00 17.77      1MBC  93
ATOM      7  CG2 VAL     1      -5.962  16.191  15.584  1.00 19.17      1MBC  94
ATOM      8  N   LEU     2      -1.328  14.772  16.218  1.00 13.50      1MBC  95
ATOM      9  CA  LEU     2      -0.529  13.847  17.019  1.00 11.36      1MBC  96
ATOM     10  C   LEU     2      -1.183  13.755  18.420  1.00  9.99      1MBC  97
ATOM     11  O   LEU     2      -1.582  14.772  18.921  1.00  8.99      1MBC  98
ATOM     12  CB  LEU     2       0.983  14.248  17.119  1.00 10.10      1MBC  99
ATOM     13  CG  LEU     2       1.692  14.001  15.751  1.00  9.73      1MBC 100
ATOM     14  CD1 LEU     2       1.216  14.865  14.716  1.00  8.79      1MBC 101
ATOM     15  CD2 LEU     2       3.147  14.217  16.051  1.00  9.54      1MBC 102
ATOM     16  N   SER     3      -1.114  12.521  18.854  1.00  9.53      1MBC 103
ATOM     17  CA  SER     3      -1.383  12.274  20.256  1.00 10.47      1MBC 104
ATOM     18  C   SER     3      -0.208  12.829  21.090  1.00 10.05      1MBC 105
ATOM     19  O   SER     3       0.833  13.076  20.589  1.00  9.70      1MBC 106
ATOM     20  CB  SER     3      -1.596  10.794  20.556  1.00 10.87      1MBC 107
ATOM     21  OG  SER     3      -0.346  10.023  20.222  1.00 11.48      1MBC 108
ATOM     22  N   GLU     4      -0.513  12.922  22.391  1.00 11.12      1MBC 109
ATOM     23  CA  GLU     4       0.423  13.415  23.392  1.00 11.78      1MBC 110
ATOM     24  C   GLU     4       1.495  12.367  23.459  1.00 11.72      1MBC 111
```

The first running index is over the number of the atom, the second running index is over the amino acid index. The third index is the atom name. In our first exercise we shall be interested in the CA-s only. The alpha carbons (CA) are at the center of the main chain of the protein. All the different amino acids (named at the fourth column) have the same backbone …N-CA-C… and the CA is at the center of it.
Column 5 lists the index of the amino acid.
Columns 6-7 have the x,y,z coordinate of the corresponding atom.

We shall be interested (at least at the beginning) in a reduced representation of protein structures that will include only CA-s.

Note also that some proteins have more than a single chain. A TERminal line indicates the end of a chain
TER 1070 ARG A 141

In this exercise we use only the first chain in a file.
We need a subroutine that will extract from a protein data bank only the CA of the first chain.
The functions crd and word (that are discussed below are rather complex and at present we shall not discuss them in details. You may use it as is, or dig into MATLAB help file to understand all of its tricks.

Below is a MATLAB routine that performs this function

```
function crd = pickCA(pdbFileName)

% Read CA protein data from pdb text file.
%

fid = fopen(pdbFileName);     % Open coordinate file
Eline = fgetl(fid);        % Skip till you get to ATOM lines
word = words(Eline); % word-break the line to words separated by space
% ~ is a logical not. Read next line if ~ TER and ~ ATOM
while (and(~strcmp(word{1},'TER'),~strcmp(word{1},'ATOM')))
   Fline = fgetl(fid);        % The first atom is N
   word = words(Fline);
end
% if TER end of chain
if (strcmp(word{1},'TER')) break; end;
Fline = fgetl(fid);        % The second atom is CA
word = words(Fline);

%special protein data bank cases are handled below
if or(strcmp(word{5},'R') ,strcmp(word{5},'A'))
   x=7; y=8; z=9;
else
   x=6; y=7; z=8;
end

i =0;

while ~strcmp(word{1},'TER');
         %fprintf(fid_out,'%80s \n',Fline);
   i = i+1;          % The first atom is CA
coords(i,:) =
[str2double(word{x}),str2double(word{y}),str2double(word{z})];
   while (~strcmp(word{1},'TER'));
            Fline = fgetl(fid);        % Find the CA of the next amino
acid
      word = words(Fline);
      if strcmp(word{1},'TER') break; end;
      if ~strcmp(word{1},'ATOM') break; end;
      if strcmp(word{3},'CA') break; end;
   end
   if or(strcmp(word{1},'TER'),~strcmp(word{1},'ATOM')) break; end;
end
fclose(fid);

crd = coords(1:i,:);
```

```
function word = words(string)

% Break a string into whitespace delimited words.
% Produces a cell-array of strings.  Individual strings are
% accessed via s{1}, s{2}, and s{3}.  Note the curly braces.

s = size(string,2);        % Length of input string
blanks = find(isspace(string));     % Find indices of all whitespace
zblanks = [0 blanks];         % 0 counts as whitespace, too
n = size(zblanks,2);       % Number of words (includes length 0)
length = [blanks s+1] - zblanks - 1;   % Lengths of all words
result = cell(1,n);        % Reserve space
for i = 1:n          % Copy all words (includes length 0)
   result{1,i} = string(zblanks(i)+1:zblanks(i)+length(i));
end
word = result(length > 0);    % Remove length 0 words
```

To read the CA from a protein structure to a MATLAB array do the following:
Connect to www.rcsb.org and extract a protein structure of interest.
Read the file by a call for the above function, in the command window of Matlab.

For example (extracting HUMAN GRANULOCYTE MACROPHAGE COLONY STIMULATING FACTOR with a protein-data-bank (pdb) code – 1gmf:

```
coor = pickCA('Z:\ron\structures\1gmf.pdb');
```

coor is a two dimensional array (1:n,1:3). The column is the number of the amino acid and the rows are the x,y,z coordinates

To plot the sequence of CA as a curve in 3D dimension we do:

```
plot3(coor(:,1),coor(:,2),coor(:,3))
```

Note that the ":" picks the complete range of the vector and there is no need to know or specify the exact dimension.

The distances between sequential CA in proteins are fixed at approximately 3.8 angstrom, making the connected picture more reasonable.

For many purposes it is useful to set the geometric center of the protein at the origin of the coordinate system (for example, applying rotation matrix on a system that is not at the origin will have a translation component). The geometric center is defined

$$\left(X_{gc},Y_{gc},Z_{gc}\right)=\frac{1}{N}\sum_{i=1}^{N}\left(X_i,Y_i,Z_i\right)$$

In our case the summation is over the coordinates of the CA. A short MATLAB script that set the geometric center of the molecule to zero is below:

```
n = size(coor,1);
gc = [sum(coor(:,1)) sum(coor(:,2)) sum(coor(:,3))]/n
for i=1:n
   coor(i,:) = coor(i,:)-gc;
end
```

By clicking on the right top bottom it is possible to rotate the protein chain in 3D. It is not that easy to understand properties of the structure from the 3D view. For example, can you identify how many helices are in the structure?

It is useful to have other representations (less straightforward) of the structure that are simpler to analyze. One interesting representation (in 2D) is the contact matrix. If the distance between a pair of amino acids i and j is less than seven, the contact matrix is set to one. Otherwise it is set to zero

$$C_{ij} = \begin{cases} 0 & r_{ij} > 7 \\ 1 & r_{ij} \le 7 \end{cases}$$

A short MATLAB script that prepares and draws a contact map is below:

```
n = size(coor,1);
counter = 0;
for i=1:n
   cont(i:i) = 0;
   for j=i+1:n
      dist = norm(coor(i,:)-coor(j,:));
      if (dist<=7)
         counter = counter + 1;
         x(counter) = i;
         y(counter) = j;
      end
   end
end
   plot(x,y,'bd')
```

We repeat the same exercise for the protein myoglobin (1mbco). Can you suggest a fingerprint for a helix? Beta sheet? Can you identify sharp turns? Explain the off-diagonal elements and what structural features they correspond to.

Homework 2:
We define the distance between two structures as the norm of the vector differences. The distance between protein structures with coordinate vectors coor1(:,1:3) and coor2(:,1-3) is norm(coor1-coor2). In this exercise we compute the distances between different representations of the same protein. Your report should include the programs, plots and explanations of the results as requested below.

1. Extract the coordinates of the protein 1LAP from the protein data bank
2. Read the CA coordinates of this protein. Plot the chain of the CA-s and the contact matrix. Assign secondary structures. You may also use the plot3 facility.
3. Instead of the CA-s it is possible to read the N atoms. Modify the code to read the N-s instead of the CA-s. Be careful not to lose any N! Stored the coordinates in a different array from the CA array. Compute the distance between the N vector representation of the protein chain and the CA vector of the protein. Repeat the process after placing the geometric centers of the two protein presentations at the origin. Any changes after the shifts of the geometric centers?