How To Use FitNumDifMR.m

1. Verify that FitNumDifMR.m is the appropriate template file to use
   a. The data points must be of the form $\left(x_1, x_2, \cdots, x_{n_s}, \hat{y}_1, \cdots, \hat{y}_{n_r}\right)$
   b. The model being fit to those data must be of the following form

$$y_1 = f_1\left(u_1, u_2, \cdots, u_{n_u}, x_{1,}, x_2, \cdots, x_{n_s}\right)$$
$$y_2 = f_2\left(u_1, u_2, \cdots, u_{n_u}, x_{1,}, x_2, \cdots, x_{n_s}\right)$$
$$\vdots$$
$$y_{n_r} = f_{n_r}\left(u_1, u_2, \cdots, u_{n_u}, x_{1,}, x_2, \cdots, x_{n_s}\right)$$

   where the u_i are found by solving a set of differential equations of the following form:

   i.

$$\frac{du_1}{dv} = g_1\left(v, u_1, u_2, \cdots, u_{n_u}, \theta_1, \theta_2, \cdots, \theta_{n_p}; x_1, x_2, \cdots, x_{n_s}\right); \quad u_1(0) = u_1^0$$
$$\frac{du_2}{dv} = g_2\left(v, u_1, u_2, \cdots, u_{n_u}, \theta_1, \theta_2, \cdots, \theta_{n_p}; x_1, x_2, \cdots, x_{n_s}\right); \quad u_2(0) = u_2^0$$
$$\vdots$$
$$\frac{du_{n_u}}{dv} = g_{n_u}\left(v, u_1, u_2, \cdots, u_{n_u}, \theta_1, \theta_2, \cdots, \theta_{n_p}; x_1, x_2, \cdots, x_{n_s}\right); \quad u_{n_u}(0) = u_{n_u}^0$$

   ii. and $\underline{u}^0$ may include the set variables, $\underline{x}$.
2. Save a copy of FitNumDifMR.m as *newname*.m in the current MATLAB working directory or in a directory that is in the MATLAB search path ("*newname*" should be some meaningful file name)
3. Change the function declaration statement to match the filename from step 2
   a. from: `function FitNumDifMR(p_guess)`
   b. to: `function newname(p_guess)`
4. Find the comment indicating the location of the first required file modification
   a. Replace
      i.
      ```
      % EDIT HERE (Required modification 1 of 4):
            % define universal and experimental constants here
      ```
   b. With statements defining variables and assigning their values for each constant that appears in the problem being solved. Universal constants like the ideal gas constant should be defined here, as well, and all the values should have consistent units.
5. Find the comment indicating the location of the second required modification and replace it with a statement defining a matrix named x
   a. There should be one row in the matrix x for each data point in the data set being fit
   b. There should be one column in the matrix x for each set variable in the data set
   c. The matrix x should contain the values of the corresponding set variables and data points

6. Find the comment indicating the location of the third required modification and replace it with a statement defining a matrix named y_hat
   a. There should be one row in the matrix y_hat for each data point in the data set being fit
   b. There should be one column in the matrix y_hat for each response variable in the data set
   c. The matrix y_hat should contain the values of the corresponding measured responses for the data points
7. Find the comment indicating the location of the fourth required file modification and change the lines that follows the comment
   a. from:

```
dudv = [
    % Evaluate du1/dv = g1(v,u(1),...,u(n);p(1),...,p(n_par)) here
    % Evaluate du2/dv = g2(v,u(1),...,u(n);p(1),...,p(n_par)) here
    % and so on through gn, one per line
];
```

   b. so that the first line within the square brackets evaluates the function g_1 in step 1.b.i, the second line evaluates the function g_2 in step 1.b.i, and so on.
   c. If the parameters or set variables are needed in order to evaluate the functions, g, they are available in the column vectors p and x_set, respectively.
8. Find the comment indicating the location of the fifth required file modification and change the line that follows the comment
   a. from:

```
v0 = ; % insert the independent variable initial value here
u0 = [
    % insert the initial values of dependent variables u1 here
    % insert initial values for u2, u3, ..., one per line
];
vf = ; % insert the independent variable final value here
```

   b. so that the initial and final values of the independent variable for data point i are assigned to v0 and vf, respectively, and
   c. so that the first line within the square brackets calculates $u_1(0)$ from the equations in step 1.b.i, the second line calculates $u_2(0)$, and so on.
   d. If the set variables or response variables are needed in order to calculate the guesses they are available in the column vectors x_set and y_hat, respectively.
9. Find the comment indicating the location of the sixth and final required file modification and change the line that follows the comment
   a. from:

```
y(i,:) = [
    % evaluate response variable y(1) here
    % evaluate response variable y(2) here
    % and so on, one response variable per line
];
```

b. so that the first line within the square brackets evaluates the function f_1 from step 1b, the second line within the square brackets evaluates the function f_2, and so on.
c. If the set variables are needed in order to evaluate the functions, $\underline{f}$, they are available in the column vectors `x_set`.

10. If the ODEs in step 1.b.i are stiff, change the solver from ode45 to ode15s
11. Save the modified version of newname.m (where newname is the filename chosen in step 2)
12. Create a column vector named `p_guess` in the MATLAB workspace; it should contain guesses for the values of the parameters, $\underline{\theta}$, one per row
13. Execute the file by typing the following at the MATLAB command prompt (again using “newname” to represent the filename chosen in step 2): `newname(p_guess)`
14. A column vector named `pf` and containing the fitted parameters will be listed in the MATLAB command window
15. The following figures will be displayed
    a. A parity plot for each of the response variables
    b. Residuals plots for each response variable plotted separately versus each set variable
16. Copy the values of `pf` to `p_guess` and repeat step 13
    a. Repeat this step until the values returned as `pf` equal the values in `p_guess` and none of the other returned quantities have changed indicating a converged minimization
17. To search for a different minimum of the objective function, repeat steps 12 through 16 using a significantly different `p_guess` in step 12