How To Use FitNumAlgSR.m

1. Verify that FitNumAlgSR.m is the appropriate template file to use
   a. The data points must be of the form $\left(x_1, x_2, \cdots, x_{n_s}, \hat{y}\right)$
   b. The model being fit to those data must be of the form $y = f\left(u_1, u_2, \cdots, u_{n_u}, x_1, x_2, \cdots, x_{n_s}\right)$ where the u_i are found by solving a set of algebraic model equations of the following form:

      i.
$$\begin{aligned} g_1\left(u_1, u_2, \cdots, u_{n_u}, \theta_1, \theta_2, \cdots, \theta_{n_p}; x_1, x_2, \cdots, x_{n_s}\right) &= 0 \\ g_2\left(u_1, u_2, \cdots, u_{n_u}, \theta_1, \theta_2, \cdots, \theta_{n_p}; x_1, x_2, \cdots, x_{n_s}\right) &= 0 \\ &\vdots \\ g_{n_u}\left(u_1, u_2, \cdots, u_{n_u}, \theta_1, \theta_2, \cdots, \theta_{n_p}; x_1, x_2, \cdots, x_{n_s}\right) &= 0 \end{aligned}$$

2. Save a copy of FitNumAlgSR.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 FitNumAlgSR(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 column vector named `y_hat`
   a. There should be one row in the `y_hat` for each data point in the data set being fit and it should contain the corresponding value of the measured response for that data point
7. Find the comment indicating the location of the fourth required file modification and change the lines that follows the comment

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a. from:

i.
```
g = [
    % evaluate g1(u(1),...,u(n);p(1),...,p(n_par)) here
    % evaluate g2(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, f, 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:

i.
```
u_guess = [
    % insert/calculate guess for u(1) here
    % insert/calculate guess for u(2) here
    % and so on, one u(i) per line
  ];
```

b. so that the first line within the square brackets calculates a guess for the value of u_1 that solves the model equations in step 1.b.i, the second line calculates a guess for the value of u_2, and so on.

c. 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) = ; % insert statement(s) to calculate y for data point i`

b. so that it evaluates the function f in step 1b and sets `y(i)` equal to the result

c. If the set variables are needed in order to evaluate the function, f, they are available in the column vectors `x_set`.

10. Save the modified version of newname.m (where newname is the filename chosen in step 2)

11. 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

12. 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)`

13. The following quantity will be listed in the MATLAB command window

a. `r_squared` - the correlation coefficient for the fit

14. The following quantities will be returned
    a. `pf` - a column vector containing the fitted parameters
    b. `pf_u` - a column vector containing the ± 95% confidence limits for the fitted parameters
    c. `y` - a column vector containing the values of the response variable predicted by the fitted model
15. The following figures will be displayed
    a. If there is one set variable per data point
        i. A model plot
    b. If there are two or more set variables per data point
        i. A parity plot
        ii. A set of residuals plots with each of the set variables as the abscissa
16. Copy the values of `pf` to `p_guess` and repeat step 12
    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 11 through 16 using a significantly different `p_guess` in step 11