Final Exam Solutions
Administered: Friday, December 8, 2017
40 points

For each problem part: 0 points if not attempted or no work shown,
1 point for partial credit, if work is shown,
2 points for correct numerical value of solution

Problem 1. (12 points)
A cylindrical aluminum rod, of diameter, *d*, and length *L*, is horizontally suspended between two heat reservoirs, which maintain the temperature at one end (z=0) at 400 K and at the other end (z=l) at 800 K. Between them a fan flows on the rod to conduct heat away. The steady state heat equation describing this set up is given below as

$$0 = \frac{k_c}{\rho C_p}\frac{d^2T}{dz^2} - \frac{h}{\rho C_p}\frac{A}{V}\left(T - T_{surr}\right)$$

where

- k_c is the thermal conductivity, $k_c = 237.0\frac{W}{m \cdot K}$
- ρ is the mass density, $\rho = 2700.0\frac{kg}{m^3}$
- C_p is the specific heat capacity, $C_p = 896.9\frac{J}{kg \cdot K}$
- d is the diameter of the rod, $d = 0.025\,m$
- l is the length of the rod, $l = 0.5\,m$
- A is the surface area of the rod, $A = \pi d l$
- V is the volume of the rod, $V = \frac{\pi}{4}d^2 l$
- A/V is the surface area to volume ratio of the rod, $A/V = \frac{4}{d}$
- T_{surr} is the surrounding temperature, $T_{surr} = 300\,K$
- h is an emprical heat transfer coefficient, $h = 40.0\frac{W}{m^2 \cdot K}$

Answer the following questions and perform the following tasks.

(a) Is this ODE problem linear or nonlinear?
(b) Is this ODE problem an initial value problem or a boundary value problem?
(c) Convert this second order ODE into a system of two first order ODEs.
(d) Find the initial temperature gradient at $z = 0$.
(e) Sketch the temperature profile.
(f) Verify that your discretization resolution was sufficient.

Solution

(a) Is this ODE problem linear or nonlinear?

The problem is linear.

(b) Is this ODE problem an initial value problem or a boundary value problem?

This problem is a boundary value problem because both conditions are not given at the same value of the independent variable, *z*.

(c) Convert this second order ODE into a system of two first order ODEs.

This conversion follows a three step process.

Step 1. Define new variables.

$$y_1 = T \qquad y_2 = \frac{dT}{dz}$$

Step 2. Write ODEs for the new variables.

In this transformation, the first equation is always

$$\frac{dy_1}{dz} = y_2$$

The second equation is substituting the variables in Step 1 into the original ODE.

$$0 = \frac{k_c}{\rho C_p}\frac{d^2T}{dz^2} - \frac{h}{\rho C_p}\frac{A}{V}\left(T - T_{surr}\right)$$

or

$$\frac{k_c}{\rho C_p}\frac{d^2T}{dz^2} = \frac{h}{\rho C_p}\frac{A}{V}\left(T - T_{surr}\right)$$

$$\frac{d^2T}{dz^2} = \frac{\rho C_p}{k_c}\frac{h}{\rho C_p}\frac{A}{V}\left(T - T_{surr}\right) = \frac{h}{k_c}\frac{A}{V}\left(T - T_{surr}\right)$$

$$\frac{dy_2}{dz} = \frac{h}{k_c}\frac{A}{V}\left(y_1 - T_{surr}\right)$$

Step 3. Write initial conditions for the new variables.

$$y_1(z=0)=T(z=0)=400 \qquad y_2(z=0)=\left.\frac{dT}{dz}\right|_0 \text{ (not given)}$$

(d) Find the initial temperature gradient at $z = 0$.
(e) Sketch the concentration profile.
(f) Verify that your discretization resolution was sufficient.

This is a boundary value problem. I used as the starting points the two Matlab functions, rk4n.m and nrnd1.m, distributed on the course website in the odesolver_bvp folder.

I modified the input file for rk4n.m, which uses the classical fourth-order Runge-Kutta method to solve a system of n ODEs.

```
function dydx = funkeval(x,y);
h = 40.0; % W/m^2/K
kc = 237.0; % W/m/K
d = 0.025; % m
AoV = 4.0/d; % 1/m
Tsurr = 300.0; % K
con = h/kc*AoV; % 1/m^2
dydx(1) = y(2);
dydx(2) = con*(y(1)-Tsurr);
```

I also modified the input for nrnd1.m, which uses the Newton Raphson method with numerical derivatives,

```
function f = funkeval(x)
xo = 0.0;
yo_1 = 400.0;
yo_2 = x;
xf = 0.5;
yf = 800.0;
n = 1000;
[x,y]=rk4n(n,xo,xf,[yo_1,yo_2]);
yf_calc = y(n+1,1);
f = yf_calc-yf;
```

At the command line prompt, I needed an initial guess for the initial slope. I used the average slope as my initial guess.

```
>> average_slope = (800 - 400)/0.5
average_slope =   800

>> [x0,err] = nrnd1(average_slope)
```

This command generated the following output:

```
icount = 1 xold = 8.000000e+02 f = 1.204599e+03 df = 1.286062e+00 xnew = -1.366572e+02  err = 1.000000e+02
icount = 2 xold = -1.366572e+02 f = 4.636013e-08 df = 1.286062e+00 xnew = -1.366572e+02  err = 2.637851e-10
```

```
x0 = -136.6572
err =   2.6379e-10
```

The code converged because the error was less than the stated tolerance of 10^{-6}. The initial slope is

$$\left.\frac{dT}{dz}\right|_0 = -136.6572\frac{\mathrm{K}}{\mathrm{m}}$$

We can run the Runge Kutta code with this initial condition to generate the result.

```
>> [x,y]=rk4n(1000,0,0.5,[400,-136.6572]);
>> y_n1000   = y(1001,1)

y_n1000 =   800.0000
```

When we use 1000 intervals in the Runge Kutta code, we obtain a temperature at the far end of the rod of 800.0 K. That matches our specified boundary condition.

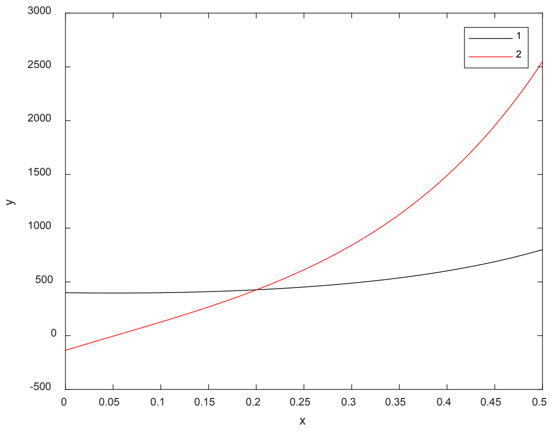
In order to verify that the spatial discretization was sufficiently fine, we also use 10,000 intervals in the Runge Kutta code. For this finer resolution, we obtain a concentration at the far end of the

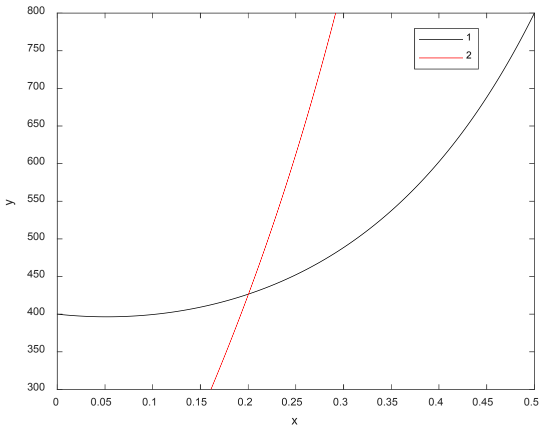
```
>> [x,y]=rk4n(10000,0,0.5,[400,-136.6572]);
>> y_n10000   = y(10001,1)

y_n10000 =   800.0000
```

The two results agree, so we had a good discretization resolution.

A plot of the profile is shown below. The black line marked “1” is the temperature. The red line marked “2” is the temperature gradient.

A second plot is also shown which zooms in on the temperature. It is clear that there is sufficient cooling that the temperature actually drops below 400 near the lower temperature reservoir.





Problem 2. (8 points)

The Hall-Petch equation states that the yield strength, σ_y, varies with grain size, *d*, according to

$$\sigma_y = \sigma_o + k_y \frac{1}{\sqrt{d}} \tag{1}$$

where σ_o and k_y are material-specific parameters.

[Materials Science and Engineering: An Introduction, 5th Edition, William D. Callister, John Wiley & Sons, Inc., New York, 2000, p. 167.]

For the σ_y vs *d* data given in the file, http://utkstair.org/clausius/docs/mse301/data/xm4p02_f17.txt, perform the following tasks. The grain size is given in mm and the yield strength in MPa.

(a) Identify all variables, $y = mx + b$, when equation (1) is linearized.

(b) Report the best value of σ_o and k_y.

(c) Report the standard deviations of σ_o and k_y.

(d) Report the measure of fit.

Solution

(a) Identify all variables, $y = mx + b$, when equation (1) is linearized.

$$y = \sigma_y, \; x = \frac{1}{\sqrt{d}}, \; m = k_y, \; b = \sigma_o$$

(b) Report the best value of σ_o and k_y.

(c) Report the standard deviations of σ_o and k_y.

(d) Report the measure of fit.

I wrote the following script, xm4p02_f17.m, in Matlab.

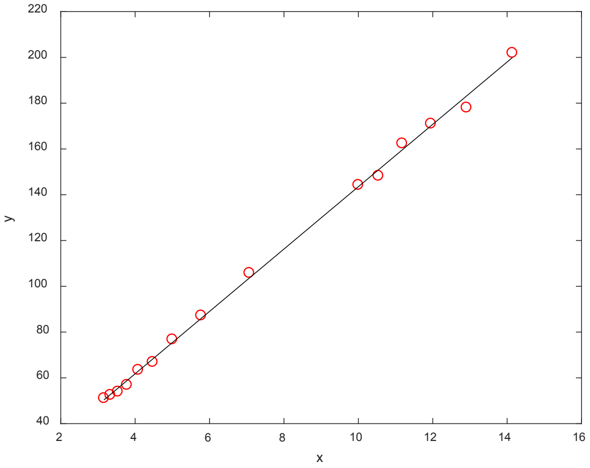
```
clear all;
format long;

M = [0.005  201.9489013
0.006   178.0468464
0.007   171.0262776
...
0.09    52.51625732
0.10    51.10776758];

n = max(size(M));
for i = 1:1:n
    x(i) = 1.0/sqrt(M(i,1));
    y(i) = M(i,2);
end
[b,bsd,MOF] = linreg1(x, y)
```

At the command line prompt, I executed the script.

```
>> xm4p02_f17
```

This generated the following output.

```
b =
   7.300962399000085
  13.621538163504301

bsd =
   1.240382815384292
   0.149070422363958

MOF =    0.998445472657267
```



Thus

(b) Report the best value of σ_o and k_y.

$\sigma_o = 7.30$ MPa $\qquad k_y = 13.62$ MPa·m$^{1/2}$

(c) Report the standard deviations of σ_o and k_y.

The standard deviations of these two parameters are

$\sigma_o = 1.24$ MPa $\qquad k_y = 0.15$ MPa·m$^{1/2}$

(d) Report the measure of fit.

MOF = 0.998

Problem 3. (12 points)

The addition of impurities into a metal to improve mechanical properties is known as solid solution strengthening. [Materials Science and Engineering: An Introduction, 5th Edition, William D. Callister, John Wiley & Sons, Inc., New York, 2000, p. 168.] Consider the following data for aluminum and indium solid solutions in magnesium [The Elastic Properties of Magnesium Solid Solutions, D. Hardie, *Acta Metallurgica* Vol. 19, 1971, pp. 719-723]

Aluminum			**Indium**		
sample #	ΔE/atomic %	(ΔE/atomic %)^2	sample #	ΔE/atomic %	(ΔE/atomic %)^2
1	-20.00	400.00	1	-34.37	1181.64
2	-3.33	11.11	2	-23.64	558.68
3	-10.00	100.00	3	-26.39	696.37
4	-10.00	100.00			
sum	-43.33333333	611.1111111		-84.40025253	2436.691768

ΔE = change in Young's modulus relative to pure Mg (kgf/mm^2)

(a) Compute the sample mean of the change in Young's Modulus/atomic % for both metals.
(b) Compute the sample variance of the change in Young's Modulus/atomic % for both metals.
(c) What PDF is appropriate for determining a confidence interval on the difference of means?
(d) Find the lower limit on a 98% confidence interval on the difference of means.
(e) Find the upper limit on a 98% confidence interval on the difference of means.
(f) Translate your result from (d) and (e) into a statement a non-statistician can understand.

Solution:

(a) Compute the sample mean of the change in Young's Modulus/atomic % for both metals.

$$\left(\frac{\Delta E}{at\%}\right)_{Al} = \frac{1}{4}\sum_{i=1}^{4}\left(\frac{\Delta E}{at\%}\right)_i = \frac{-43.33}{4} = -10.83 \text{ kgf/mm}^2\text{/at\%}$$

$$\left(\frac{\Delta E}{at\%}\right)_{In} = \frac{1}{3}\sum_{i=1}^{3}\left(\frac{\Delta E}{at\%}\right)_i = \frac{-84.40}{3} = -28.13 \text{ kgf/mm}^2\text{/at\%}$$

(b) Compute the sample variance of the change in Young's Modulus/atomic % for both metals.

$$\text{var}\left(\frac{\Delta E}{at\%}\right)_{Al} = \frac{n\sum_{i=1}^{n}\left(\frac{\Delta E}{at\%}\right)_i^2 - \left(\sum_{i=1}^{n}\left(\frac{\Delta E}{at\%}\right)_i\right)^2}{n(n-1)} = 47.22 \text{ (kgf/mm}^2\text{/at\%)}^2$$

$$\text{var}\left(\frac{\Delta E}{at\%}\right)_{In} = \frac{n\sum_{i=1}^{n}\left(\frac{\Delta E}{at\%}\right)_i^2 - \left(\sum_{i=1}^{n}\left(\frac{\Delta E}{at\%}\right)_i\right)^2}{n(n-1)} = 31.11 \text{ (kgf/mm}^2\text{/at\%)}^2$$

(c) What PDF is appropriate for determining a confidence interval on the difference of means?

We must use the t-distribution to determine the confidence interval on the difference of means when the population variance is unknown.

(d) Find the lower limit on a 98% confidence interval on the difference of means.
(e) Find the upper limit on a 98% confidence interval on the difference of means.

$$\alpha = \frac{1 - C.I.}{2} = \frac{1 - 0.98}{2} = 0.01$$

$$v = \frac{\left(\frac{s_1^2}{n_1} + \frac{s_2^2}{n_2}\right)^2}{\left[\left(\frac{s_1^2}{n_1}\right)^2 \Big/ (n_1 - 1)\right] + \left[\left(\frac{s_2^2}{n_2}\right)^2 \Big/ (n_2 - 1)\right]} \quad \text{if } \sigma_1 \neq \sigma_2$$

$$v = 4.91 \approx 5$$

The limits on the t-distribution are given by

```
>> t = icdf('t',0.01,5)

t =  -3.364929998907217
```

and for the upper limit

```
>> t = icdf('t',0.99,5)

t =   3.364929998907217
```

We next insert all of these numbers into the equation for the confidence interval on the difference of means.

$$P\left[\left(\overline{X}_1 - \overline{X}_2\right) + t_\alpha \sqrt{\frac{s_1^2}{n_1} + \frac{s_2^2}{n_2}} < (\mu_1 - \mu_2) < \left(\overline{X}_1 - \overline{X}_2\right) + t_{1-\alpha} \sqrt{\frac{s_1^2}{n_1} + \frac{s_2^2}{n_2}}\right] = 1 - 2\alpha$$

$$P\left[\begin{array}{l} (-10.83 - -28.13) + \text{-}3.3649\sqrt{\frac{47.22}{4} + \frac{31.11}{3}} \\ \quad < (\mu_1 - \mu_2) < (-10.83 - -28.13) + 3.3649\sqrt{\frac{47.22}{4} + \frac{31.11}{3}} \end{array}\right] = 0.98$$

$$P[1.454 < (\mu_1 - \mu_2) < 33.146] = 0.98$$

(f) Translate your result from (d) and (e) into a statement a non-statistician can understand.

We are 98% sure that the change in Young's Modulus per atomic % of impurity of aluminum is between 1.454 and 33.146 kgf/mm^2/at% greater than that for indium. In this case since both impurities resulted in a reduction in the Young's Modulus relative to pure magnesium, this means that aluminum reduced the Young's Modulus less than indium by the above amount.

Problem 4. (8 points)

Consider the van der Waal's equation of state,

$$p = \frac{RT}{V-b} - \frac{a}{V^2}$$

Consider argon at T=120 K and p = 200,000 Pa. The van der Waals constants for argon are a=0.1381 m^6/mol^2 and b=3.184×10^{-5} m^3/mol. The gas constant is R=8.314 J/mol/K.

(a) Is this algebraic equation linear or nonlinear in the molar volume?
(b) What is the appropriate technique to solve this equation?
(c) Find the liquid molar volume.
(d) Find the vapor molar volume.

Solution:

(a) Is this algebraic equation linear or nonlinear in the molar volume?

This equation is nonlinear in the molar volume.

(b) What is the appropriate technique to solve this equation?

One appropriate technique is to use the Newton-Raphson method with numerical approximations to the derivative.

(c) Find the liquid molar volume.
(d) Find the vapor molar volume.

First we modify the input function in nrnd1.m

```
function f = funkeval(x)
V = x; % m^3/mole
p = 200000.0; % Pa
T = 120.0; % K
R = 8.314; % J/mol/K
a = 0.1381;
b = 3.184e-5;
f = R*T/(V-b) - a/V^2 - p;
```

For the liquid molar volume, we know that root must be just a little bigger than b, so we guess

```
>> b = 3.184e-5;
>> V_guess = 1.1*b

V_guess =     3.5024e-05

>> [V,err] = nrnd1(V_guess)

icount = 1 xold = 3.502400e-05 f = 2.005615e+08 df = -9.318667e+13 xnew = 3.717625e-05  err = 1.000000e+02
icount = 2 xold = 3.717625e-05 f = 8.684029e+07 df = -2.983050e+13 xnew = 4.008738e-05  err = 7.261947e-02
```

```
icount = 3 xold = 4.008738e-05 f = 3.483270e+07 df = -1.041402e+13 xnew = 4.343217e-05  err = 7.701179e-02
icount = 4 xold = 4.343217e-05 f = 1.265496e+07 df = -4.062936e+12 xnew = 4.654690e-05  err = 6.691602e-02
icount = 5 xold = 4.654690e-05 f = 3.897530e+06 df = -1.877967e+12 xnew = 4.862230e-05  err = 4.268408e-02
icount = 6 xold = 4.862230e-05 f = 8.335765e+05 df = -1.142022e+12 xnew = 4.935221e-05  err = 1.478987e-02
icount = 7 xold = 4.935221e-05 f = 7.087259e+04 df = -9.575593e+11 xnew = 4.942623e-05  err = 1.497460e-03
icount = 8 xold = 4.942623e-05 f = 7.889091e+02 df = -9.405074e+11 xnew = 4.942706e-05  err = 1.697071e-05
icount = 9 xold = 4.942706e-05 f = 1.835471e+00 df = -9.403158e+11 xnew = 4.942707e-05  err = 3.949198e-08

V =      4.942706686059153e-05
err =      3.949198246957197e-08
```

The error is less than our specified tolerance of 10^{-6}, so the code converged. The liquid molar volume is 4.94×10^{-5} m^3/mole.

An initial guess for the vapor molar volume is the ideal gas law.

```
>> p = 200000.0; % Pa
T = 120.0; % K
R = 8.314; % J/mol/K
>> V_guess = R*T/p

V_guess =   0.0049884

>> [V,err] = nrnd1_xm4p04_f17(V_guess)

icount = 1 xold = 4.988400e-03 f = -4.264959e+03 df = -3.838839e+07 xnew = 4.877300e-03  err = 1.000000e+02
icount = 2 xold = 4.877300e-03 f = 9.453048e+01 df = -4.011662e+07 xnew = 4.879656e-03  err = 4.829013e-04
icount = 3 xold = 4.879656e-03 f = 5.363240e-02 df = -4.007876e+07 xnew = 4.879657e-03  err = 2.742354e-07

V =   0.004879657499075
err =      2.742354456891266e-07
```

The error is less than our specified tolerance of 10^{-6}, so the code converged. The vapor molar volume is 4.88×10^{-3} m^3/mole.

An alternate solution method would be to remember that the van der Waal's equation of state is a cubic polynomial that can be expressed as

$$pV^3 - (pb + RT)V^2 + aV - ab = 0$$

Then we can use the Matlab intrinsic roots function to obtain all three roots of the cubic polynomial.

```
>>  p = 200000.0; % Pa
T = 120.0; % K
R = 8.314; % J/mol/K
a = 0.1381;
b = 3.184e-5;
>> coeffs = [p,-p*b-R*T,a,-a*b];
>> Vvec = roots(coeffs)

Vvec =
   0.004879657499203
   0.000091155433932
   0.000049427066865
```

These largest and smallest of these roots match the results obtained from the Newton-Raphson process.