Test III - Fall 2006 - Solutions

Note Title 12/9/2006

Problem I

```
z = [40 38 31; 51 46 39; 65 53 48; 72 67 56]
[x, y] = meshgrid([1 2 3], [1 2 3 4])
% or
%   x = [1 2 3; 1 2 3; 1 2 3; 1 2 3]
%   y = [1 1 1; 2 2 2; 3 3 3; 4 4 4]
% or make them columns already:
%   x = [1 1 1 1 2 2 2 2 3 3 3 3]
%   y = [1 2 3 4 1 2 3 4 1 2 3 4]

M = [x(:).^0 x(:) y(:)]
b = z(:)
MyCoefs = M\b
% or
%    fSSR = inline('sum((zdata - (a(1)+a(2)*xdata+a(3)*ydata)).^2)',...
%        'a', 'xdata', 'ydata', 'zdata')
%    [MyCoefs, Sr] = fminsearch(@(alpha)fSSR(alpha, x(:), y(:), z(:)), [1 1
1])

A = MyCoefs(1)
B = MyCoefs(2)
C = MyCoefs(3)

zhat = A + B*x + C*y
St = sum((z(:)-mean(z(:))).^2)
Sr = sum((z(:)-zhat(:)).^2)
r2 = (St-Sr) / St

[xm, ym] = meshgrid(linspace(1, 3, 20), linspace(1, 4, 20))
zm = A + B*xm + C*ym
surfc(xm, ym, zm)
xlabel('x')
ylabel('y')
zlabel('z')
```

Problem II

(1)

```
clear
x = (1:5)'
y = [1.0489 1.1910 1.4122 1.6910 2.0000]'
fSSR1 = inline('sum((yd-a(1)*exp(a(2)*xd)).^2)', 'a', 'xd', 'yd')
[aloc1, Sr1] = fminsearch(@(a)fSSR1(a,x,y),[1 1])
fSSR2 = inline('sum((yd-a(1)*xd.^a(2)).^2)', 'a', 'xd', 'yd')
[aloc2, Sr2] = fminsearch(@(a)fSSR2(a,x,y),[1 1])
fSSR3 = inline('sum((yd-a(1).*xd./(a(2)+xd)).^2)', 'a', 'xd', 'yd')
[aloc3, Sr3] = fminsearch(@(a)fSSR3(a,x,y),[1 1])

% Note - code below note required for test
% Used to calculate values for table in part 2
St = sum((y-mean(y)).^2)
r21 = (St - Sr1) / St
yhat1 = aloc1(1)*exp(aloc1(2)*x)
r22 = (St - Sr2) / St
yhat2 = aloc2(1)*x.^aloc2(2)
r23 = (St - Sr3) / St
yhat3 = aloc3(1).*x./(aloc3(2)+x)
```

(2) $St = \sum (y-\bar{y})^2$ so

$$\bar{y} = \frac{1}{5}(1.0489 + 1.1910 + 1.4122 + 1.6910 + 2.0000) = 1.4686$$

$$\begin{array}{rrrrr} 1.0489 & 1.1910 & 1.4122 & 1.6910 & 2.0000 \\ -1.4686 & -1.4686 & -1.4686 & -1.4686 & -1.4686 \end{array}$$

$$(-.4197)^2 + (-.2776)^2 + (-.0564)^2 + (.2224)^2 + (.5314)^2 = \boxed{.5882}$$

$r^2 = (St - Sr) / St$ so

$$Sr = \sum (y - \hat{y})^2$$

$$\begin{array}{rrrrr} 1.0489 & 1.1910 & 1.4122 & 1.6910 & 2.0000 \\ -1.0232 & -1.2089 & -1.4283 & -1.6875 & -1.9937 \end{array}$$

$$(.0257)^2 + (-.0179)^2 + (-.0161)^2 + (.0035)^2 + (.0063)^2 = .001292$$

$$r^2 = (.5882 - .001292)/.5882 = \boxed{.9978}$$

$\boxed{\text{Exponential is numerically best since its } r^2 \text{ is closest to 1}}$

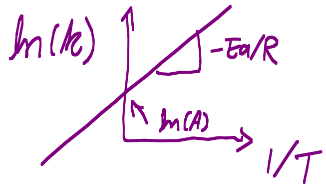
Problem III

(1) With exponentials, use natural logs

$$k = A e^{-Ea/RT}$$

$$\ln(k) = \ln(A e^{-Ea/RT}) = \ln(A) + \ln(e^{-Ea/RT})$$

$$\ln(k) = \ln(A) - \frac{Ea}{R}\left(\frac{1}{T}\right)$$



(2)

$$\begin{bmatrix} | & | \\ 1 & 1./T \\ | & | \end{bmatrix} \begin{bmatrix} \ln(A) \\ -Ea/R \end{bmatrix} = \begin{bmatrix} | \\ \ln(k) \\ | \end{bmatrix}$$

(others are also possible)

$$\begin{bmatrix} 1 & 0.00137 \\ 1 & 0.00132 \\ 1 & 0.00127 \\ 1 & 0.00123 \end{bmatrix} \begin{bmatrix} \ln(A) \\ -Ea/8.314 \end{bmatrix} = \begin{bmatrix} -3.352 \\ -2.254 \\ -1.070 \\ -0.237 \end{bmatrix}$$

(3)

```
T = [730 760 790 810]'
k = [0.035 0.105 0.343 0.789]'
% Model:
% ln(k) = -(Ea/R)*(1/T) + ln(A)*(1)
M = [1./T T.^0]
b = log(k);
MyCoefs = M\b
% or
%     MyCoefs = polyfit(1./T, log(k), 1)
Ea = -8.314 * MyCoefs(1)
A = exp(MyCoefs(2))

khat = A*exp(-Ea/8.314./T)
% or
%     khat = exp(polyval(MyCoefs, 1./T))

St = sum((k-mean(k)).^2)
Sr = sum((k-khat).^2);
r2 = (St-Sr) / St
```

Problem IV

(1) T=480 is closest to 500, so using NN, $Cp(480) \approx cp(500) = 35.15 \frac{kJ}{kmol\cdot K}$

(2) T=480 is between 450 & 500, so using linear

$$Cp(480) = cp(450) + \frac{cp(500) - cp(450)}{500-450}(480-450)$$

$$Cp(480) = 33.35 + \frac{1.8}{50}(30) = \boxed{34.43 \frac{kJ}{kmol\cdot K}}$$

(3) for $500 \leq T \leq 550$, $Cp(T) = Cp(500) + \frac{Cp(550) - Cp(500)}{550 - 500}(T-500)$

$$Cp(T) = 35.15 + 0.0442(T-500) \quad \underline{or} \quad \boxed{13.05 + .0442T}$$

(4)

```
clear
T = 400:50:600
cp = [31.96 33.35 35.15 37.36 40.05]

P = polyfit(T, cp, 4)
alpha   = P(5);
beta    = P(4);
gamma   = P(3);
delta   = P(2);
epsilon = P(1);

dT = T(2) - T(1);
dcdTfirst = (-cp(3)+4*cp(2)-3*cp(1))/(2*dT)
dcdTlast  = (3*cp(5)-4*cp(4)+cp(3))/(2*dT)


Tm = linspace(400, 600, 50)
cpC = spline(T, [dcdTfirst cp dcdTlast], Tm)
cpNK = spline(T, cp, Tm)
% or
%    cpNK = interp1(T, cp, Tm, 'spline')
```

(5)

$$\left.\frac{dcp}{dT}\right|_{400} = \frac{-Cp(500) + 4Cp(450) - 3cp(400)}{2\cdot 50} = \frac{-35.15 + 133.4 - 95.88}{100} = \boxed{0.0237 \frac{kJ}{kmol-K^2}}$$

$$\left.\frac{dcp}{dt}\right|_{600} = \frac{3Cp(600) - 4Cp(550) + Cp(500)}{2\cdot 50} = \frac{120.15 - 149.44 + 35.15}{100} = \boxed{0.0586 \frac{kJ}{kmol-K^2}}$$

Problem V

(1) $\Delta T = 4$

$$\int_0^0 a(\tau)\,d\tau = 0$$

$$\int_0^4 a(\tau)\,d\tau = \frac{4}{2}\left(0.75 + 1.75\right) = 5$$

$$\int_0^8 a(\tau)\,d\tau = \frac{4}{3}\left(0.75 + 4(1.75) + 3.00\right) = 14.\overline{3}$$

$$\int_0^{12} a(\tau)\,d\tau = 4\cdot\frac{3}{8}\left(0.75 + 3(1.75+3) + 6.50\right) = 32.25$$

$$\int_0^{16} a(\tau)\,d\tau = \int_0^8 a(\tau)\,d\tau + \int_8^{16} a(\tau)\,d\tau = 14.\overline{3} + \frac{4}{3}\left(3 + 4(6.5) + 8\right) = 63.\overline{6}$$

$$\int_0^{20} a(\tau)\,d\tau = \int_0^8 a(\tau)\,d\tau + \int_8^{20} a(\tau)\,d\tau = 14.\overline{3} + 4\cdot\frac{3}{8}\left(3 + 3(6.5+8) + 1.5\right) = 86.\overline{3}$$

$$\int_0^{24} a(\tau)\,d\tau = \int_0^{16} a(\tau)\,d\tau + \int_{16}^{24} a(\tau)\,d\tau = 63.\overline{6} + \frac{4}{3}\left(8 + 4(1.5) - 5.5\right) = 75$$

$$\int_0^{28} a(\tau)\,d\tau = \int_0^{16} a(\tau)\,d\tau + \int_{16}^{28} a(\tau)\,d\tau = 63.\overline{6} + 4\cdot\frac{3}{8}\left(8 + 3(1.5 - 5.5) - 8\right) = 45.\overline{6}$$

$$\int_0^{32} a(\tau)\,d\tau = \int_0^{24} a(\tau)\,d\tau + \int_{24}^{32} a(\tau)\,d\tau = 75 + \frac{4}{3}\left(-5.5 + 4(-8) - 6\right) = 17$$

$$\int_0^{36} a(\tau)\,d\tau = \int_0^{24} a(\tau)\,d\tau + \int_{24}^{36} a(\tau)\,d\tau = 75 + 4\cdot\frac{3}{8}\left(-5.5 + 3(-8-6) - 2.5\right) = 0$$

(2) $\int_0^{36} v(\tau)\,d\tau$: 9 Areas so use 3 Simp 1/3 and 1 Simp 3/8:

$$\frac{4}{3}\left(0 + 4(5 + 32.35 + 86.\overline{3}) + 2(14.\overline{3} + 63.\overline{6}) + 75\right) + 4\cdot\frac{3}{8}\left(75 + 3(45.\overline{6} + 17) + 0\right)$$

$$= 967.64 + 394.5 = 1362\ \frac{\text{miles}}{\text{hr}}\cdot\text{sec}$$

$$1362\ \frac{\text{miles}}{\text{hr}}\cdot\text{sec}\cdot\left(\frac{\text{hr}}{3600\ \text{sec}}\right) = \boxed{0.378\ \text{miles}}$$