Homework #10

Name: Andrea Livingston

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CBE660: Intermediate Problems in Chemical and Biological Engineering - Fall 2016

Department of Chemical and Biological Engineering, University of Wisconsin-Madison

Problem 1. Solve Exercise 4.33.
Let $X_i = 1, 2, ..., n$ be statistically independent, normally distributed random variables with zero mean and unit variance. Consider the random variable Y to be the sum of squares $Y = X_1^2 + X_2^2 + ... + X_n^2$.

4.33.a Find Y's probability density. This density is known as the χ^2 density with n degrees of freedom, and we say $Y \sim \chi_n^2$. Show that the mean of this density is n.

4.33.b Repeat for the random variable $Z = \sqrt{X_1^2 + X_2^2 + ... + X_n^2}$. This density is known as the χ density with n degrees of freedom.

Solution:

4.33.a
Chi-Squared Distribution

Begin with the normally distributed variable X. The pdf for a normally distributed variable is

$$f_X(x) = \frac{1}{\sqrt{2\pi}\sigma} exp\left[\frac{-(x-\sigma)^2}{2\sigma^2}\right]$$

For a mean of zero and the variance of one this becomes

$$f_X(x) = \frac{1}{\sqrt{2\pi}} exp\left[\frac{-x^2}{2}\right]$$

If we let $Y = X^2$ then Y also has a chi-squared distribution with one degree of freedom.

$$f(y) = y = x^2$$
$$f^{-1}(y) = x = \sqrt{(y)}$$

Using the change of variables equation (equation 4.23)

$$f_Y(y) = f_X(f^{-1}(y)) \left| det\frac{df^{-1}(y)}{dy} \right|$$

$$\left| det\frac{df^{-1}(y)}{dy} \right| = \frac{d}{dy}y^{1/2} = \frac{1}{2\sqrt{y}}$$

$$f_Y(y) = f_X(\sqrt{y})\frac{1}{2\sqrt{y}}$$

But because $\pm x$ gives the same results

$$f_Y(y) = f_X(\sqrt{y})\frac{1}{2\sqrt{y}} + f_X(-\sqrt{y})\frac{1}{2\sqrt{y}}$$

$$f_X(\sqrt{y}) = f_X(-\sqrt{y}) = \frac{1}{\sqrt{2\pi}} exp\left[\frac{-y}{2}\right]$$

$$f_Y(y) = \frac{1}{\sqrt{2\pi}} exp\left[\frac{-y}{2}\right]\frac{1}{2\sqrt{y}} + \frac{1}{\sqrt{2\pi}} exp\left[\frac{-y}{2}\right]\frac{1}{2\sqrt{y}}$$
$$f_Y(y) = \frac{1}{\sqrt{2\pi y}} exp\left[\frac{-y}{2}\right]$$

Given the characteristic function for X, the characteristic function of a one-dimensional Y can be found

$$\varphi_X(t) = E\left[e^{itx}\right] = \int_{-\infty}^{\infty} e^{itx} f_X(x)dx$$
$$\varphi_Y(t) = \int_{-\infty}^{\infty} e^{ity} f_Y(y)dy$$
$$\varphi_Y(t) = \int_{-\infty}^{\infty} e^{ity} \frac{1}{\sqrt{2\pi y}} exp\left[\frac{-y}{2}\right] dy$$
$$\varphi_Y(t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{ity} \frac{1}{\sqrt{y}} exp\left[\frac{-y}{2}\right] dy$$
$$\varphi_Y(t) = \frac{1}{\sqrt{1-2it}}$$

Now expanding this to an n-dimensional case using the property for $\eta = \epsilon_1 + \epsilon_2 + \ldots \epsilon_n$ (equation 4.8)

$$\varphi_\eta(t) = \varphi_{\epsilon_1}(t)\varphi_{\epsilon_2}(t)\ldots\varphi_{\epsilon_n}(t)$$

and defining $Y = \Sigma_{i=1}^n X_i^2$ the characteristic equation becomes

$$\varphi_Y(j\omega) = \frac{1}{(1-2it)^{\frac{n}{2}}}$$

Moving from the characteristic function back to the probability density (equation on p.354)

$$f_Y(y) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-ity}\varphi_Y(t)dt$$
$$f_Y(y) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-ity}\frac{1}{(1-2it)^{\frac{n}{2}}}dt$$

Defining the gamma function

$$\Gamma(z) = \int_0^{\infty} x^{z-1}e^{-x}dx$$
$$\Gamma(\frac{n}{2}) = \int_0^{\infty} y^{\frac{n}{2}-1}e^{-\frac{n}{2}}dy$$

Taking the inverse transform of the characteristic function gives the n-dimensional χ^2 probability density for $y \geq 0$. For $y < 0$ then $f_Y(y) = 0$

$$f_Y(y) = \frac{1}{2^{n/2}\Gamma(n/2)} y^{n/2-1}e^{-y/2}$$

4.33.b
CHI DISTRIBUTION

For the chi distribution, we now consider $Z = \sqrt{\sum_{i=1}^{n}(\frac{X_i - \mu_i}{\sigma_i})^2} = \sqrt{x}$. Beginning with the χ^2 probability density

$$f_Y(y) = \frac{1}{2^{n/2}\Gamma(n/2)} y^{n/2-1} e^{-y/2}$$

Apply the change of variables formula with the mapping relationship $z = y^2$ and $y = \sqrt{z}$.

$$g(z) = f(y)\frac{dy}{dz} = f(z^2)2z$$

$$g(z) = f_Z(z) = \frac{2z}{2^{n/2}\Gamma(n/2)}(z^2)^{n/2-1}e^{-z^2/2}$$

$$f_Z(z) = \frac{2z^1 z^{n-2} e^{-z^2/2}}{2^{n/2}\Gamma(n/2)}$$

Simplifying $z^1 z^{n-2} = z^{n-1}$ and $\frac{2}{2^{n/2}} = n^{1-n/2}$ gives the Chi probability density

$$f_Z(z) = \frac{2^{1-n/2} z^{n-1} e^{-z^2/2}}{\Gamma(n/2)}$$

Problem 2. Solve Exercise 4.31.

A common model for the temperature dependence of the reaction rate is the Arrhenius model. In this model the reaction rate (rate constant, k) is given by

$$k = k_0 exp(-E/T)$$

in which the parameter k_0 is the preexponential factor, E is the activation energy scaled by the gas constant, and T is the temperature in Kelvin. We wish to estimate k_0 and E from the measurements of the reaction rate at different temperatures. In order to use linear least squares, we take the logarithm of the reaction rate

$$ln(k) = ln(k_0) - E/T$$

Assume you have made measurements of the rate constant at 10 temperatures evenly distributed between 300 and 500K. Model the measurement process as the true value plus measurement error, e, which is distributed normally with zero mean and 0.001 variance. Choose the true value of the parameters to be $ln(k_0) = 1$, $E = 100$.

4.31.a Generate a set of experimental data for this problem. Estimate the parameters from these data using least squares. Plot the data and the model fit using both (T,k) and (1/T, ln k) as the (x,y) axes.

4.31.b Calculate the 95% confidence intervals for your parameter estimates. What are the coordinates of the semi-major axes of the ellipse corresponding to the 95% confidence interval?

4.31.c What are the coordinates of the corners of the box corresponding to the 95% confidence interval?

4.31.d Plot your results by showing the parameter estimate, ellipse and box. Are the parameter estimates highly correlated? Why or why not?

Solution:

4.31.1

Experimental data was generated according to

$$ln(k) = lnk_0 - E/T + e$$

$$ln(k) = 1 - 100/T + e$$

Using the least squares regression, the parameters for k_0 and E were fitted.The fitted results were plotted against the 'experimental' data.

$$x_{ls} = (A^T A)^{-1} A^T b$$

4.31.b

The 95% confidence interval was determined using $\chi^2(n_p = 2, 0.95)$. Solving this equation

$$(x - m)^T P^{-1}(x - m) \le \chi^2(n_p, \alpha)$$

leads to

$$|\hat{\theta} - \theta_0|_i \le \left(\chi^2(n_p, \alpha)\sigma^2(X^T X)^{-1}_{ii}\right)^{1/2}$$

and

$$c_i = (\chi^2(n_p, \alpha)\sigma^2(A^T A)^{-1}_{ii})^{1/2}$$

The resultant confidence intervals were

$$ln(k) = 1.000 \pm 0.1508$$

$$E = 100.1211 \pm 57.15$$

4.31.c

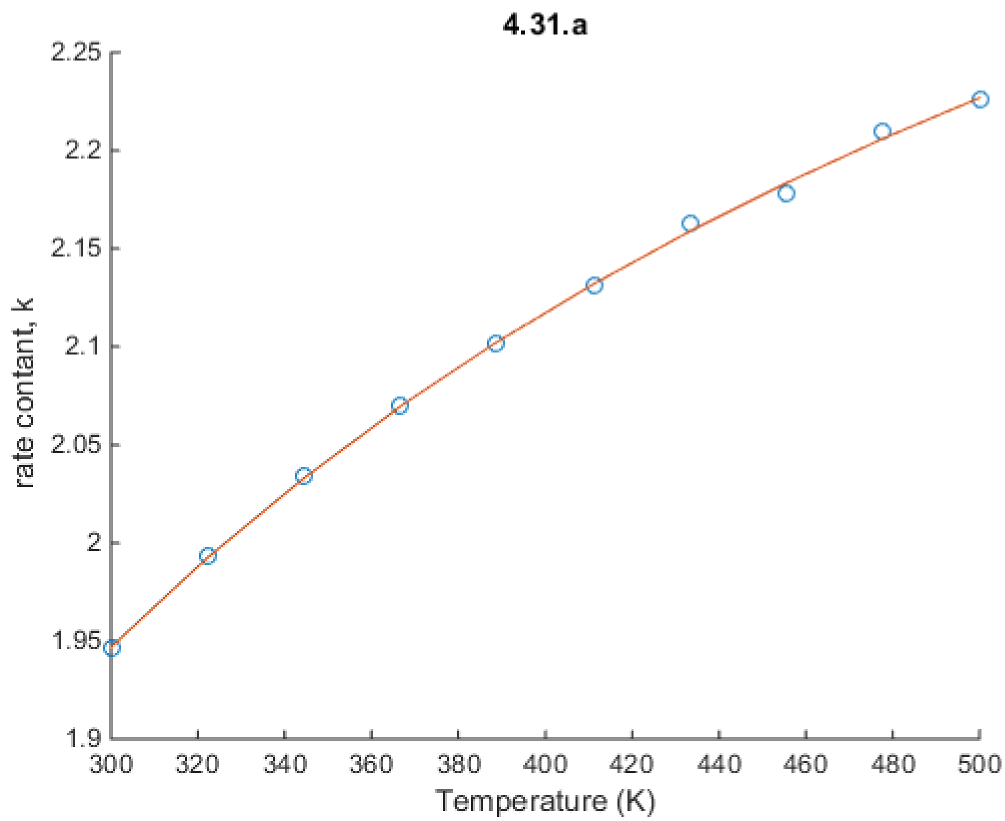
The corresponding corners of the bounding box are given by

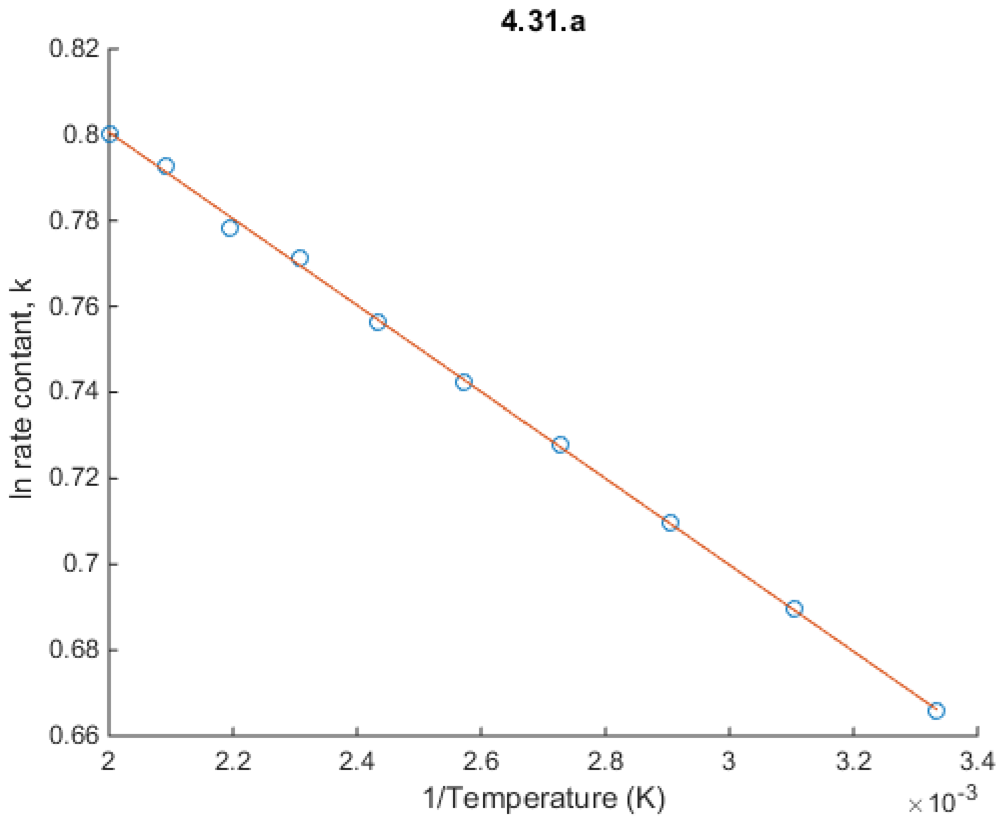
$$1.148791 \;\; 1.58080e+02$$

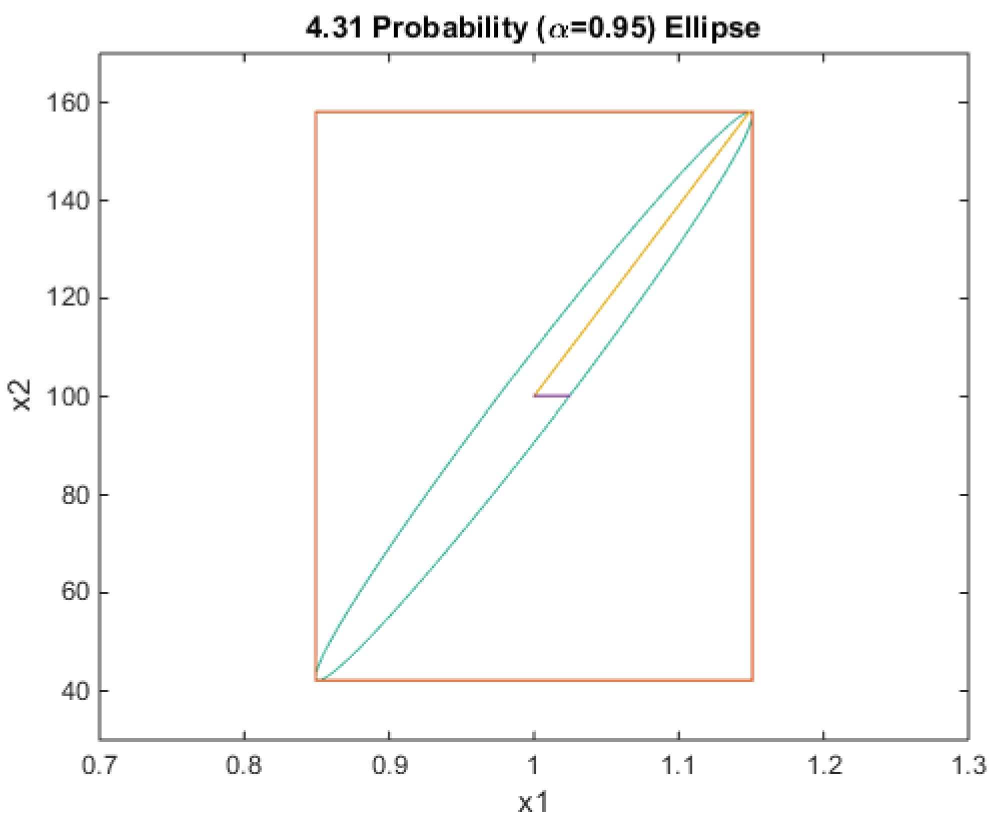
$$1.024507 \;\; 1.00121e+02$$

4.31.d

Yes, the system is highly coordinated.Changing one variable would change the covariance matrix which would have a significant impact on the other.








```
clear all

T=linspace(300,500,10) ;
ln_k0=1 ;
```

```
E=100 ;
var=0.001

for i=1:length(T)

    %generate e
    e=normrnd(0,var);

    %calculate the rate constant
    ln_k(i,1)=ln_k0-E/T(i)+e;
    k(i)=exp(ln_k(i)) ;

    %Set up least squares
    A(i,1)=1 ;
    A(i,2)=-1./T(i) ;
end

x_ls=inv(A'*A)*A'*ln_k ;

ln_k_ls=x_ls(1)-x_ls(2)./T ;
k_ls=exp(ln_k_ls) ;

figure(1)
scatter(T,k)
hold on
plot(T,k_ls)
    title('4.31.a')
    xlabel('Temperature (K)')
    ylabel('rate contant, k')

figure(2)
scatter(1./T,ln_k)
hold on
plot(1./T ,log(k_ls))
    title('4.31.a')
    xlabel('1/Temperature (K)')
    ylabel('ln rate contant, k')



% Chi-squared distribution
P=var*inv(A'*A) ;
chi2=chi2inv(0.95,2) ;
c1=sqrt(P(1,1)*chi2) ;
c2=sqrt(P(2,2)*chi2) ;

[v,l]=eig(inv(P)) ;
v1=-sqrt(chi2/l(1,1))*v(:,1)+x_ls ;
v2=-sqrt(chi2/l(2,2))*v(:,2)+x_ls ;

% Ellipse
figure(3)
```

```
syms x1 x2
x=[x1; x2]-x_ls ;
f=x'*inv(P)*x==chi2 ;
ezplot(f,[0.7,1.3,30,170])
hold on
plot(x_ls(1),x_ls(2))
    title('4.31 Probability (\alpha=0.95) Ellipse')
    xlabel('x1')
    ylabel('x2')

% Bounding Box
box1=[-c1+x_ls(1), c1+x_ls(1), c1+x_ls(1), -c1+x_ls(1), -c1+x_ls(1)];
box2=[c2+x_ls(2), c2+x_ls(2), -c2+x_ls(2), -c2+x_ls(2), c2+x_ls(2)] ;
hold on
plot(box1,box2)

% Vectors
hold on
plot([x_ls(1) v1(1)],[x_ls(2) v1(2)])
hold on
plot([x_ls(1) v2(1)],[x_ls(2) v2(2)])
```

Problem 3. Solve Exercise 4.22.

Given the normally distributed random variable $\xi \in \mathbb{R}^n$, consider the random variable, $\eta \in \mathbb{R}^n$, obtained by the linear transformation

$$\eta = A\xi$$

in which A is a nonsingular matrix. Using the result on transforming probability densities show that if $\xi \sim N(m, P)$, then $\eta \sim N(Am, APA^T)$. This result establishes that invertible linear transformations of nonsingular normal random variables are normal.

Solution:

Considering the random variable η transformed as

$$\eta = A\xi$$

Given that this is a linear transformation, we can say

$$\eta = f(\xi)$$

$$\xi = f^{-1}(\eta)$$

$$\eta = A\xi$$

$$\xi = A^{-1}\eta$$

Because the variable associated with η is y and the variable associated with ξ is x

$$x = A^{-1}y$$

From equation 4.23

$$p_\eta(y) = p_\xi(f^{-1}(y)) \left| det \frac{dA^{-1}\eta}{d\eta} \right|$$

Taking the derivative with respect to η

$$p_\eta(y) = p_\xi(f^{-1}(y)) \left| det\ A^{-1} \right|$$

Simplifying the determinant term using properties of linear algebra

$$det(A^{-1}) = \frac{1}{det(A)}$$

$$p_\eta(y) = p_\xi(f^{-1}(y)) \frac{1}{det\ A}$$

By inspection $|x| = \sqrt{x\,x}$. Extending this concept to the determinants, which are scalars

$$p_\eta(y) = p_\xi(f^{-1}(y)) \sqrt{\frac{1}{det\ A} \frac{1}{det\ A}}$$

From equation 4.12 for the probability density of $\xi \sim N(m, P)$ where m is the mean and P is a real, symmetric positive definite matrix (covariance matrix of ξ)

$$p_\xi(x) = \frac{1}{(2\pi)^{n/2}(det\ P)^{1/2}} exp\left[\frac{-1}{2}(x-m)^T P^{-1}(x-m) \right]$$

$$p_\xi(f^{-1}(y)) = p_\xi(A^{-1}y) = \frac{1}{(2\pi)^{n/2}(det\ P)^{1/2}} exp\left[\frac{-1}{2}(A^{-1}y - m)^T P^{-1}(A^{-1}y - m)\right]$$

Substituting $p_\xi(f^{-1}(y))$ into the expression for $p_\eta(y)$

$$p_\eta(y) = \sqrt{\frac{1}{det\ A}\frac{1}{det\ A}}\ \ \frac{1}{(2\pi)^{n/2}(det\ P)^{1/2}} exp\left[\frac{-1}{2}(A^{-1}y - m)^T P^{-1}(A^{-1}y - m)\right]$$

$$p_\eta(y) = \sqrt{\frac{1}{det\ A}\frac{1}{det\ A}\frac{1}{(2\pi)^n(det\ P)}} exp\left[\frac{-1}{2}(A^{-1}y - m)^T P^{-1}(A^{-1}y - m)\right]$$

Introducing the identity matrix $I = A^{-1}A$ and rearranging

$$p_\eta(y) = \sqrt{\frac{1}{det\ A}\frac{1}{det\ A}\frac{1}{(2\pi)^n(det\ P)}} exp\left[\frac{-1}{2}(I(A^{-1}y - m))^T P^{-1}(I(A^{-1}y - m))\right]$$

$$p_\eta(y) = \sqrt{\frac{1}{det\ A}\frac{1}{det\ A}\frac{1}{(2\pi)^n(det\ P)}} exp\left[\frac{-1}{2}(A^{-1}A(A^{-1}y - m))^T P^{-1}(A^{-1}A(A^{-1}y - m))\right]$$

$$p_\eta(y) = \sqrt{\frac{1}{det\ A}\frac{1}{det\ A}\frac{1}{(2\pi)^n(det\ P)}} exp\left[\frac{-1}{2}(A^{-1}(AA^{-1}y - Am))^T P^{-1}(A^{-1}(AA^{-1}y - Am))\right]$$

$$p_\eta(y) = \sqrt{\frac{1}{det\ A}\frac{1}{det\ A}\frac{1}{(2\pi)^n(det\ P)}} exp\left[\frac{-1}{2}(A^{-1}(y - Am))^T P^{-1}(A^{-1}(y - Am))\right]$$

$$p_\eta(y) = \sqrt{\frac{1}{det\ A\ (det\ P)\ det\ A}}\frac{1}{(2\pi)^{n/2}} exp\left[\frac{-1}{2}(y - Am)^T A^{-1T} P^{-1} A^{-1}(y - Am)\right]$$

Now let $det(A) = det(A^T)$ and $A^{-1T}P^{-1}A^{-1} = (APA^T)^{-1}$

$$p_\eta(y) = \frac{1}{(2\pi)^{n/2} det\ (APA^T)^{1/2}} exp\left[\frac{-1}{2}(y - \mathbf{Am})^T (\mathbf{APA^T})^{-1}(y - \mathbf{Am})\right]$$

Comparing this equation to equation 4.12 for $p_\xi(x)$ for which $\xi \sim N(m, P)$

$$p_\xi(x) = \frac{1}{(2\pi)^{n/2}(det\ P)^{1/2}} exp\left[\frac{-1}{2}(x - \mathbf{m})^T \mathbf{P}^{-1}(x - \mathbf{m})\right]$$

we can draw parallels to see that $\eta \sim N(Am, APA^T)$