Homework Assignment Number Eleven Solutions

Problem 1.
Consider the normal distribution

$$f(x;\mu,\sigma)=\frac{1}{\sqrt{2\pi}\sigma}e^{-\frac{1}{2}\left(\frac{x-\mu}{\sigma}\right)^2}$$

This function does not have an analytical integral.

For the standard normal distribution, where the mean is zero and the standard deviation is one, evaluate the integral from x = -2.0 to 1.0, i.e. $p(-2.0 \le x \le 1.0)$, using

(a) the trapezoidal method with 1 interval.
(b) the trapezoidal method with 10 intervals.
(c) the trapezoidal method with 100 intervals.
(d) the trapezoidal method with 1000 intervals.
(e) the Simpson's Second Order method with 100 intervals.
(f) the Simpson's Second Order method with 1000 intervals.
(g) the Simpson's Third Order method with 99 intervals.
(h) the Simpson's Fourth Order method with 100 intervals.
(i) Gaussian quadrature of sixth order.
(j) the cdf command in MatLab.
(k) Comment on the effect of number of intervals and order of the method.

Solution:

In each code, whether it be trapezoidal.m, simpson2.m, simpson3.m, simpson4.m or gaussquad.m, the integrand is input as

```
function f = funkeval(x)
f = 1/sqrt(2.0*pi)*exp(-0.5*x^2);
```

(a) the trapezoidal method with 1 interval.

```
>>   integral = trapezoidal(-2.0,1.0,1)
integral =   0.443942536548497
```

(b) the trapezoidal method with 10 intervals.

```
>> integral = trapezoidal(-2.0,1.0,10)
integral =   0.815965728062905
```

(c) the trapezoidal method with 100 intervals.

```
>> integral = trapezoidal(-2.0,1.0,100)
```

```
integral =   0.818568367248082
```

(d) the trapezoidal method with 1000 intervals.

```
>> integral = trapezoidal(-2.0,1.0,1000)
integral =   0.818594351655828
```

(e) the Simpson’s Second Order method with 100 intervals.

```
>> integral = simpson2(-2.0,1.0,100)
integral =   0.818594615812413
```

(f) the Simpson’s Second Order method with 1000 intervals.

```
>> integral = simpson2(-2.0,1.0,1000)
integral =   0.818594614120533
```

(g) the Simpson’s Third Order method with 99 intervals.

```
>> integral = simpson3(-2.0,1.0,99)
integral =   0.818594618084208
```

(h) the Simpson’s Fourth Order method with 100 intervals.

```
>> integral = simpson4(-2.0,1.0,100)
integral =   0.818594614119623
```

(i) Gaussian quadrature of sixth order.

```
>> integral = gaussquad(-2.0,1.0,6)
integral =   0.818594704229380
```

(j) the cdf command in MatLab.

```
>> plow = cdf('normal',-2.0,0,1)
plow =   0.022750131948179

>> phigh = cdf('normal',1.0,0,1)
phigh =   0.841344746068543

>> p = phigh - plow
p =   0.818594614120364
```

(k) Comment on the effect of number of intervals and order of the method.

As the number of intervals increases, the accuracy of the method increases. As the order of the method increases, the number of intervals needed to generate a given level of accuracy drastically decreases.

Problem Two.
Consider the van der Waals equation of state.

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

where P is pressure (Pa), T is temperature (K), $\underline{V}$ is molar volume (m^3/mol), R is the gas constant (8.314 J/mol/K = 8.314 Pa*m^3/mol/K), a is the van der Waal's attraction constant (0.2303 Pa*m^6/mol^2 for methane) and b is the van der Waal's repulsion constant (4.306×10^{-5} m^3/mol for methane).
The entropy change upon expanding is

$$\Delta S = \int_{\underline{V}_1}^{\underline{V}_2} \left(\frac{\partial P}{\partial T}\right)_{\underline{V}'} d\underline{V}'$$

where

$$\left(\frac{\partial P}{\partial T}\right)_{\underline{V}} = \frac{R}{\underline{V} - b}$$

Find the entropy change upon expanding methane from 0.05 to 0.11 m^3/mol at T = 298 K.

(a) Find analytical integral.
(b) Find the integral using Gaussian quadrature.
(c) Find the integral using the data provided in 'file.hw11p02c.txt'.
(d) Repeat part (a) at T = 398 K. Comment

Solution:

(a) Find analytical integral.

$$\Delta S = \int_{\underline{V}_1}^{\underline{V}_2} \left(\frac{\partial P}{\partial T}\right)_{\underline{V}'} d\underline{V}' = \int_{\underline{V}_1}^{\underline{V}_2} \frac{R}{\underline{V}' - b} d\underline{V}' = R \ln\left(\frac{\underline{V}_2 - b}{\underline{V}_1 - b}\right)$$

```
>> R = 8.314
>> b = 4.306e-5;
>> dS = R*log((0.11-b)/(0.05-b))

dS =   6.559142405481035 J/mol/K
```

(b) Find the integral using Gaussian quadrature.

The integrand function is given by:

```
function f = funkeval(x)
R = 8.314;
b = 4.306e-5;
f = R/(x-b);
```

```
>> integral = gaussquad(0.05,0.11,6)
integral =   6.559142375860369
```

(c) Find the integral using the data provided in 'file.hw11p02c.txt'.

When you have irregularly spaced data. You can apply the Trapezoidal rule to each interval. (I did this in excel. It could also be done in MatLab.)

Volume	dp/dT	Trapezoid
(m^3/mol)	(Pa/K)	Area
0.05	155.7688	
0.054815	157.2796	0.753655
0.060239	133.9064	0.789703
0.065479	131.0798	0.694294
0.070968	108.7339	0.658098
0.07555	118.8203	0.521391
0.080741	106.736	0.585386
0.086229	103.7671	0.57765
0.091716	97.3176	0.551674
0.096724	89.83216	0.468612
0.101642	82.4402	0.42362
0.106358	85.88743	0.396961
0.11	78.98348	0.300189
	sum	6.721234

`dS =   6.72` J/mol/K

(d) Repeat part (a) at T = 398 K. Comment.

`dS =   6.559142405481035` J/mol/K

We get the same result as in part A. The entropy change due to expansion of a van der Waal's gas is not a function of temperature.