Problem Set #2 Solutions
Estimation Exercise E2-1 (25 points)

Suppose every gallon of gasoline that was consumed in the United States since 1940 were used to heat up the top 100 meters of the world’s oceans. Estimate the resulting increase in temperature of that volume of water. Enter your answer in units of degrees Celsius.

Estimate the total amount of gas consumed in the US since 1940

The U.S. Energy Information Administration provides the total US consumption of gasoline per year. <http://www.eia.gov/dnav/pet/hist/LeafHandler.ashx?n=pet&s=mfgpus1&f=a>
These data are distributed as an excel spreadsheet.

Import the data using the appropriate filepath:

rawData = Import["Dropbox/3.016/usOilConsumption1945-2011.xls"]

(* note: this will not work unless you also have the same file in the same location *)

The portion of rawData that provides the US annual usage is buried within the data structure. To extract it, explore the sections of the data structure with Part. Note that the units are thousands of barrels per year.

datesAndBarrels = Table[{rawData[[2, i, 1]], rawData[[2, i, 2]]}, {i, 4, 70}];

ListPlot[datesAndBarrels,
  PlotLabel -> Style["Annual oil consumption", FontSize -> 24], AxesLabel ->
  {Style["Year", FontSize -> 20], Style["Oil consumption [10^3 barrels]", FontSize -> 20]}]

Annual oil consumption

Oil consumption [10^3 barrels]

The data for the WWII years 1940-1944 are absent, so a simple linear extrapolation is used to estimate the data. The data appear roughly linear up to ~1970, so the fit is done up to that point. Consumption for 2012 is not known yet, but given that the trend is dropping off in modern times, assume that January - September 2012 consumption is roughly equal to (9/12) times 2011 consumption.
The data for the WWII years 1940-1944 are absent, so a simple linear extrapolation is used to estimate the data. The data appear roughly linear up to ~1970, so the fit is done up to that point. Consumption for 2012 is not known yet, but given that the trend is dropping off in modern times, assume that January-September 2012 consumption is roughly equal to \((9/12) \times 2011\) consumption.

```
line = Fit[Take[datesAndBarrels, 25], \{1, x\}, x]
-1.00878 \times 10^8 + 52215.8 x

Show[Plot[line, \{x, 1939, 1970\}, PlotRange -> \{(1939, 2012), \{0, 4 \times 10^6\}\}],
AxesLabel -> \{Style["Year", FontSize -> 20],
Style["Oil consumption \[10^3\text{ barrels}\]", FontSize -> 20]\},
PlotStyle -> \{Red, Thick\},
PlotLabel -> Style["Annual oil consumption, with mid-century fit", FontSize -> 24]]
ListPlot[datesAndBarrels]
```

Annual oil consumption, with mid-century fit

Oil consumption \([10^3\text{ barrels}]\)

Proceeding to assemble the list of \{year, consumption\} with the extrapolated data included:
finalBarrels = Join[Table[{i, line /. x -> i}, {i, 1940, 1944}],
  datesAndBarrels, {{2012, (9/12) Last[datesAndBarrels][[2]]}}]

{1940, 420271.}, {1941, 472487.}, {1942, 524703.}, {1943, 576919.},
{1944, 629134.}, {1945, 579343.}, {1946, 722512.}, {1947, 773408.}, {1948, 834550.},
{1949, 879721.}, {1950, 954773.}, {1951, 1.08957*10^6}, {1952, 1.08099*10^6},

Next, the total consumption of gasoline, in thousands of barrels, is computed:

totGas = Sum[finalBarrels[[i, 2]], {i, Length[finalBarrels]]]

1.5457*10^6

Convert thousands of barrels to SI units: One barrel = 42 US gallons. 1 US gallon = 0.00378541 m³

metricGas = totGas 1000 x 42 x 0.00378541 (* in m³ *)
2.45747 x 10^10

Estimate how much water is in the upper 100 m of the oceans

According to NOAA, the ocean covers 71% of the Earth. The average radius of the Earth is 6371 km. The total surface area of the oceans is:

surfAreaOcean = 4 Pi (6371 x 10^3)² 0.71 (* in m² *)

3.62146 x 10^14

100 m << radius of the Earth, so we can ignore the roundness of the Earth and approximate the volume of the ocean as a planar slab. Also, ignore the shallow edges of the ocean where the depth is less than 100m, because that is such a small portion of the seas.

volToHeat = 100 surfAreaOcean

3.62146 x 10^16

Seawater has the following approximate average properties (from http://www.kayelaby.npl.co.uk/general_physics/s2_7/2_7_9.html):
salinity = 35 g/kg
density = 1025 kg/m³

cp = 3993 J/kg K
boiling point = 100.56 °C
Thus, the total mass of water is equal to the volume times the density:
\[ \text{kgWater} = \text{volToHeat} \times 1025 (\text{* kg *}) \]
\[ 3.71199 \times 10^{19} \]
And the amount of energy, in joules, required to heat this volume of seawater by 1 degree C is equal to the mass of seawater times the heat capacity of seawater:
\[ \text{unitsJperKwater} = \text{kgWater} \times 3993 (\text{* J/K *}) \]
\[ 1.4822 \times 10^{23} \]

Estimate the amount of energy released from the gasoline, and release it all into the seawater

Let's assume that the energy held in the gasoline will be released by combustion (as opposed to nuclear processes, or other chemical reactions). According to Wolfram Alpha, the heat of combustion for gasoline is \(4.5 \times 10^7 \text{ J/kg}\), and the density is \(726 \text{ kg/m}^3\).

The amount of energy released from the entire gasoline supply is equal to the density times volume times the heat of combustion:
\[ \text{gasInJoules} = 726 \text{ metricGas} \times 4.5 \times 10^7 (\text{* J *}) \]
\[ 8.02855 \times 10^{20} \]
Finally, divide the total amount of heat supplied by the gasoline (in J, above) by the number of Joules per degree temperature rise for the seawater (units J/K, obtained in the previous subsection) to get the increase in temperature of the water.
\[ \text{oceanHeating} = \text{gasInJoules} / \text{unitsJperKwater} (\text{* K *}) \]
\[ 0.00541665 \]
Stunning! If all of the gasoline burned in the United States since 1940 was used to heat the upper oceans, it would only increase the temperature by 0.005 degrees Celsius.

According to NOAA, the 21st century mean July ocean temperature is 0.62 K warmer than the 20th century mean July ocean temperature, so direct heating of the oceans by burning fossil fuel is likely not the cause of ocean warming (<http://en.wikipedia.org/wiki/Greenhouse_effect>.

Individual (Handworked) Exercise I2-1 (40 points)

The van der Waals equation is a better approximation to the equation of state of a gas than the ideal gas law. The equation of state relates the pressure, molar volume (i.e., volume per mole of gas), and temperature (P, V, and T) in terms of two material parameters, a and b. For example, a and b are tabulated for water vapor, argon, etc.

The van der Waals model predicts a critical point which is observed in every gas, whereas the ideal gas model does not have a critical point. The critical point appears on the P(T) diagram at the termination of the curve of equilibrium between the vapor and liquid phase.

The van der Waals model is:
\[(P + \frac{a}{V})(V - b) = RT\]

i. What are the units of \(a\) and \(b\)?

The units of \(P\) are force/area (SI: \(kg/s^2m\)), the units of \(V\) are volume/mole (SI: \(m^3/mol\)), and the units of \(RT\) are energy/mole (SI: \(kg m^2/s^2\)mol).

Because \(b\) is added to \(V\), it must have the same units, so the units of \(b\) are volume/mole, or \(m^3/mol\).

Similarly, \(a/V^2\) must have the same units as \(P\), so rearranging, we see that the units of \(a\) must be the same as the units of \(P \ V^2\), which are \(kg m^5/s^2\)mol\(^2\). This has units of molar energy times molar volume.

ii. Under what conditions is the model of an ideal gas the same as a van der Waals gas?

Expanding the van der Waals equation gives:

\[P \ V - P \ b + a/\ V - a \ b/ \ V^2 = RT\]

The ideal gas law is:

\[P \ V = RT\]

To get the van der Waals model to be the same, then all the other terms on the left-hand side must be negligibly small, which would happen if:

\[b \ll \ V\]

and

\[a \ll P \ V^2\]

iii. Calculate the two partial derivatives \(\partial f_P / \partial V\) and \(\partial f_P / \partial T\).

Rearranging the van der Waals equation, we have

\[P = RT/(V-b) - a/V\]

taking derivatives with respect to \(V\) and \(T\) yields

\[
\frac{\partial P}{\partial V} = 2 \ a/\ V^3 - \frac{RT}{(b - V)^2}
\]

and

\[
\frac{\partial P}{\partial T} = R/(V - b)
\]

This problem could be solved using mathematica by the following:

Define \(\text{vdwP}\) as the expression for \(P(V, T)\):
\( \text{vdwP} = \frac{RT}{(\text{molarV} - b)} + \frac{a}{\text{molarV}^2} \)

\[
\frac{a}{\text{molarV}^2} + \frac{RT}{-(b + \text{molarV})}
\]

The first derivative of pressure with respect to molar volume:

\[
\frac{dP}{dV} = \text{Simplify}[D[\text{vdwP}, \text{molarV}]]
\]

\[
\frac{2a}{\text{molarV}^3} - \frac{RT}{(b - \text{molarV})^2}
\]

And the first derivative with respect to temperature:

\[
\text{Simplify}[D[\text{vdwP}, T]]
\]

\[
\frac{R}{-(b + \text{molarV})}
\]

iv. Find expressions for the maximum, minimum, and inflection points of the isotherms of pressure (i.e., \( P = f_P(V, \ T = \text{const}) \)) so that pressure is a function of a single variable).

Maxima and minima occur where \( \frac{dp}{dV} = 0 \):

\[
2aV_c^3 - RT(b - Vc)^2 = 0
\]

Solving this equation for \( V_c \) would provide the molar volume at which \( P \) is maximized or minimized. To determine whether it is a maximum or minimum, the sign of the second derivative can be checked. If \( \frac{\partial^2 P}{\partial V^2} |_{V = V_c} > 0 \), then \( P \) is locally concave up, and this indicates the presence of a minimum. If \( \frac{\partial^2 P}{\partial V^2} |_{V = V_c} < 0 \), then this indicates the presence of a maximum. Note that this equation will have multiple solutions, but only those that are real and positive should be considered because molar volume is a positive quantity.

Inflection points occur where \( \frac{\partial^2 p}{\partial V^2} = 0 \):

\[
\frac{\partial^2 p}{\partial V^2} = RT(b - Vc)^3 \cdot \frac{6a}{Vc} = 0
\]

Solving the above equation for \( V_c \) provides the location of infection points. Again, this equation will have multiple solutions, but only those that are real and positive should be considered because molar volume is a positive quantity.

This problem could be solved using mathematica by the following:

The extrema are located at the roots of the first derivative:
\textbf{Simplify\{Solve\}[dPdV = 0, molarV]} \\
\{ molarV \rightarrow \frac{1}{3 \ R \ T} \left\{ 2 a + \\
\frac{(4 a (a + 3 b \ R \ T))}{8 a^3 + 36 a^2 b \ R \ T + 27 a b^2 R^2 T^2 + 3 \sqrt{3} \sqrt{a^2 b^3 R^3 T^3 (8 a + 27 b \ R \ T)}} \right\}^{1/3} + \\
\left\{ 8 a^3 + 36 a^2 b \ R \ T + 27 a b^2 R^2 T^2 + 3 \sqrt{3} \sqrt{a^2 b^3 R^3 T^3 (8 a + 27 b \ R \ T)} \right\}^{1/3} \right\}, \\
\{ molarV \rightarrow \frac{1}{6 \ R \ T} \left\{ -4 a + \frac{4 \left(1 + i \sqrt{3}\right) a (a + 3 b \ R \ T)}{8 a^3 + 36 a^2 b \ R \ T + 27 a b^2 R^2 T^2 + 3 \sqrt{3} \sqrt{a^2 b^3 R^3 T^3 (8 a + 27 b \ R \ T)}} \right\}^{1/3} + \\
\left\{ 1 - i \sqrt{3} \left( 8 a^3 + 36 a^2 b \ R \ T + 27 a b^2 R^2 T^2 + 3 \sqrt{3} \sqrt{a^2 b^3 R^3 T^3 (8 a + 27 b \ R \ T)} \right)^{1/3} \right\}, \\
\{ molarV \rightarrow \frac{1}{6 \ R \ T} \left\{ -4 a + \frac{4 \left(1 - i \sqrt{3}\right) a (a + 3 b \ R \ T)}{8 a^3 + 36 a^2 b \ R \ T + 27 a b^2 R^2 T^2 + 3 \sqrt{3} \sqrt{a^2 b^3 R^3 T^3 (8 a + 27 b \ R \ T)}} \right\}^{1/3} + \\
\left\{ 1 + i \sqrt{3} \left( 8 a^3 + 36 a^2 b \ R \ T + 27 a b^2 R^2 T^2 + 3 \sqrt{3} \sqrt{a^2 b^3 R^3 T^3 (8 a + 27 b \ R \ T)} \right)^{1/3} \right\} \right\} \\
\text{Note that because the derivative is cubic with } V, \text{ there are 3 solutions.}

\textbf{The inflection point(s) are located at the roots of the second derivative:}

\textbf{Simplify\{Solve\}[D[dPdV, molarV] = 0, molarV]} \\
\{ molarV \rightarrow \frac{1}{4} \left\{ -\frac{3 a}{R \ T} - \left\{ \frac{1}{(R^2 T^2)} \left( 9 a^2 + 2 \times 2^{2/3} R \ T \left( 9 a^2 b^4 R T + \sqrt{a^3 b^8 R^3 T^2 (81 a + 256 b \ R \ T)} \right) \right)^{1/3} \right\} - \frac{8 a b}{R T} \right\} - \\
\sqrt{2} \left\{ \frac{9 a^2}{R^2 T^2} \frac{24 a b}{R T} + (8 \times 2^{1/3} a b^3) \left( 9 a^2 b^4 R T + \sqrt{a^3 b^8 R^3 T^2 (81 a + 256 b \ R \ T)} \right)^{1/3} - \\
\frac{1}{R T} 2^{2/3} \left( 9 a^2 b^4 R T + \sqrt{a^3 b^8 R^3 T^2 (81 a + 256 b \ R \ T)} \right)^{1/3} + \\
\left( 9 a \left( 3 a^2 + 12 a b R T + 8 b^2 R^2 T^2 \right) \right) \sqrt{R^2 T^2} \sqrt{1/(R^2 T^2)} \left( 9 a^2 + 2 \times 2^{2/3} R \ T \left( 9 a^2 b^4 R T + \sqrt{a^3 b^8 R^3 T^2 (81 a + 256 b \ R \ T)} \right)^{1/3} \right) + \\
8 a b R T \right\} - \\
\left\{ 3 - (2 \times 2^{1/3} b^7 R T) \left( 9 a^2 b^4 R T + \sqrt{a^3 b^8 R^3 T^2 (81 a + 256 b \ R \ T)} \right)^{1/3} \right\} \right\}, \\
\{ molarV \rightarrow \frac{1}{4} \left\{ -\frac{3 a}{R \ T} - \left\{ \frac{1}{(R^2 T^2)} \left( 9 a^2 + 2 \times 2^{2/3} R \ T \left( 9 a^2 b^4 R T + \sqrt{a^3 b^8 R^3 T^2 (81 a + 256 b \ R \ T)} \right)^{1/3} \right) + \\
\right\} \right\} \right\}.
\[
8 \, a \, b \, R \, T \left( 3 - \left( 2 \times 2^{1/3} b^2 \, R \, T \right) \right) / \left( 9 \, a^2 \, b^4 \, R \, T + \sqrt{a^3 \, b^8 \, R^2 \, T^2 \left( 81 \, a + 256 \, b \, R \, T \right)} \right)^{1/3} \right) \right) + \\
\sqrt{2} \left( 9 \, a^2 \, R \, T^{2/3} + \left( 8 \times 2^{1/3} a \, b^3 \right) / \left( 9 \, a^2 \, b^4 \, R \, T + \sqrt{a^3 \, b^8 \, R^2 \, T^2 \left( 81 \, a + 256 \, b \, R \, T \right)} \right)^{1/3} \right) - \\
\frac{1}{RT} \left( 9 \, a^2 \, b^4 \, R \, T + \sqrt{a^3 \, b^8 \, R^2 \, T^2 \left( 81 \, a + 256 \, b \, R \, T \right)} \right)^{1/3} + \\
\left( 9 \, a \left( 3 \, a^2 + 12 \, a \, b \, R \, T + 8 \, b^2 \, R \, T^2 \right) \right) / \left( R^3 \, T^3 \left( 1 / \left( R^2 \, T^2 \right) \left( 9 \, a^2 + 2 \times 2^{2/3} R \, T \right) \right) \right) \left( 9 \, a^2 \, b^4 \, R \, T + \sqrt{a^3 \, b^8 \, R^2 \, T^2 \left( 81 \, a + 256 \, b \, R \, T \right)} \right)^{1/3} + 8 \, a \, b \, R \, T \\
\left( 9 \, a^2 \, b^4 \, R \, T + \sqrt{a^3 \, b^8 \, R^2 \, T^2 \left( 81 \, a + 256 \, b \, R \, T \right)} \right)^{1/3} \right) \), \{ \text{molar} V \rightarrow \frac{1}{4} \left( \frac{3 \, a}{RT} \left( 9 \, a^2 + 2 \times 2^{2/3} R \, T \right) \right) \left( 9 \, a^2 \, b^4 \, R \, T + \sqrt{a^3 \, b^8 \, R^2 \, T^2 \left( 81 \, a + 256 \, b \, R \, T \right)} \right)^{1/3} + \\
8 \, a \, b \, R \, T \left( 3 - \left( 2 \times 2^{1/3} b^2 \, R \, T \right) \right) / \left( 9 \, a^2 \, b^4 \, R \, T + \sqrt{a^3 \, b^8 \, R^2 \, T^2 \left( 81 \, a + 256 \, b \, R \, T \right)} \right)^{1/3} \right) - \\
\sqrt{2} \left( 9 \, a^2 \, R \, T^{2/3} + \left( 8 \times 2^{1/3} a \, b^3 \right) / \left( 9 \, a^2 \, b^4 \, R \, T + \sqrt{a^3 \, b^8 \, R^2 \, T^2 \left( 81 \, a + 256 \, b \, R \, T \right)} \right)^{1/3} \right) - \\
\frac{1}{RT} \left( 9 \, a^2 \, b^4 \, R \, T + \sqrt{a^3 \, b^8 \, R^2 \, T^2 \left( 81 \, a + 256 \, b \, R \, T \right)} \right)^{1/3} + \\
\left( 9 \, a \left( 3 \, a^2 + 12 \, a \, b \, R \, T + 8 \, b^2 \, R \, T^2 \right) \right) / \left( R^3 \, T^3 \left( 1 / \left( R^2 \, T^2 \right) \left( 9 \, a^2 + 2 \times 2^{2/3} R \, T \right) \right) \right) \left( 9 \, a^2 \, b^4 \, R \, T + \sqrt{a^3 \, b^8 \, R^2 \, T^2 \left( 81 \, a + 256 \, b \, R \, T \right)} \right)^{1/3} + 8 \, a \, b \, R \, T \\
\left( 9 \, a^2 \, b^4 \, R \, T + \sqrt{a^3 \, b^8 \, R^2 \, T^2 \left( 81 \, a + 256 \, b \, R \, T \right)} \right)^{1/3} \right) \), \{ \text{molar} V \rightarrow \\
\frac{1}{4RT} \left( -3 \, a + RT \left( 9 \, a^2 + 2 \times 2^{2/3} R \, T \right) \right) \left( 9 \, a^2 \, b^4 \, R \, T + \sqrt{a^3 \, b^8 \, R^2 \, T^2 \left( 81 \, a + 256 \, b \, R \, T \right)} \right)^{1/3} + \\
8 \, a \, b \, R \, T \left( 3 - \left( 2 \times 2^{1/3} b^2 \, R \, T \right) \right) / \left( 9 \, a^2 \, b^4 \, R \, T + \sqrt{a^3 \, b^8 \, R^2 \, T^2 \left( 81 \, a + 256 \, b \, R \, T \right)} \right)^{1/3} \right) + \\
\sqrt{2} \left( 9 \, a^2 \, R \, T^{2/3} + \left( 8 \times 2^{1/3} a \, b^3 \right) / \left( 9 \, a^2 \, b^4 \, R \, T + \sqrt{a^3 \, b^8 \, R^2 \, T^2 \left( 81 \, a + 256 \, b \, R \, T \right)} \right)^{1/3} \right) - \\
\frac{1}{RT} \left( 9 \, a^2 \, b^4 \, R \, T + \sqrt{a^3 \, b^8 \, R^2 \, T^2 \left( 81 \, a + 256 \, b \, R \, T \right)} \right)^{1/3} + \\
\left( 9 \, a \left( 3 \, a^2 + 12 \, a \, b \, R \, T + 8 \, b^2 \, R \, T^2 \right) \right) / \left( R^3 \, T^3 \left( 1 / \left( R^2 \, T^2 \right) \left( 9 \, a^2 + 2 \times 2^{2/3} R \, T \right) \right) \right) \left( 9 \, a^2 \, b^4 \, R \, T + \sqrt{a^3 \, b^8 \, R^2 \, T^2 \left( 81 \, a + 256 \, b \, R \, T \right)} \right)^{1/3} + 8 \, a \, b \, R \, T \\
\left( 9 \, a^2 \, b^4 \, R \, T + \sqrt{a^3 \, b^8 \, R^2 \, T^2 \left( 81 \, a + 256 \, b \, R \, T \right)} \right)^{1/3} \right) \right) \).

Individual Exercise I2-2 (15 points)

Find a simpler form of

...
\[ \frac{1}{2} \left( 2 \cos\left(\frac{\pi w}{4}\right) + \cos\left(\frac{\pi w}{4}\right)^3 \sin[p] + \cos\left(\frac{\pi w}{4}\right)^5 \sin[p] - 3 \cos[p] \cos\left(\frac{\pi w}{4}\right)^2 \sin\left(\frac{\pi w}{4}\right) + 5 \cos[p] \cos\left(\frac{\pi w}{4}\right)^4 \sin\left(\frac{\pi w}{4}\right) - 3 \cos\left(\frac{\pi w}{4}\right) \sin[p] \sin\left(\frac{\pi w}{4}\right)^2 - 10 \cos\left(\frac{\pi w}{4}\right)^3 \sin[p] \sin\left(\frac{\pi w}{4}\right)^2 + \cos[p] \sin\left(\frac{\pi w}{4}\right)^3 - 10 \cos[p] \cos\left(\frac{\pi w}{4}\right)^2 \sin\left(\frac{\pi w}{4}\right)^3 + 5 \cos\left(\frac{\pi w}{4}\right) \sin[p] \sin\left(\frac{\pi w}{4}\right)^4 + \cos[p] \sin\left(\frac{\pi w}{4}\right)^5 \right) \]

The functions Simplify or FullSimplify will distill this expression down.

\[
\]

\[
\cos\left(\frac{\pi w}{4}\right) + \cos[p w] \sin\left[p + \frac{\pi w}{4}\right]
\]

\[
\]

\[
\cos\left(\frac{\pi w}{4}\right) + \cos[p w] \sin\left[p + \frac{\pi w}{4}\right]
\]

Individual Exercise I2-3 (45 points)

i. Compute the integral \[\int \cos(\log(x)) \, dx\]

What does Mathematica do with the constant of integration (i.e., what is the value at \(x = 0\)?)

The function Integrate does an anaytical integration:

\[
\text{integrand} = \cos[\log[x]];
\]

\[
\text{integral} = \text{Integrate}[\text{integrand}, x]
\]

\[
\frac{1}{2} x \cos[\log[x]] + \frac{1}{2} x \sin[\log[x]]
\]

To find the value at \(x = 0\), we cannot simply plug in \(x = 0\) because \(\log[x]\) diverges. To see this, attempt to apply the rule \(x = 0\):

\[
\text{integral} /. x \rightarrow 0
\]

\[
\text{Interval}([0, 0])
\]

The output is not easily interprieted by humans, but the function Limit can be used to evalute the limit as \(x \rightarrow 0\).
Now it is clear that the integrand is equal to 0 when $x=0$. Therefore, the constant of integration is zero.

**ii. Plot the integral and integrand for $-1/2 \leq x \leq 10$**

```math
\text{Plot}\left[\{\text{integrand, integral}, \{x, -0.5, 10\}\right], \\
\text{PlotStyle} \to \{\{\text{Thick, Blue}, \{\text{Dashed, Thick, Red}\}\}\}
```

Out of curiosity, plot the same pair of functions over a variable range:

```math
\text{Manipulate}\left[\text{Plot}\left[\{\text{integrand, integral}, \{x, -10^{\text{scale}-1}, 10^{\text{scale}}\}\right], \\
\text{PlotStyle} \to \{\{\text{Thick, Blue}, \{\text{Dashed, Thick, Red}\}\}, \{\text{scale, 1}, -8, 5\}\}
```

The behavior near $x=0$ is difficult to see, but by considering the nature of $\cos(\log(x))$, it becomes clear that there are an infinite number of oscillations in the function between $x=1$ and $x=0$. This is because $\log(x)$ takes values $[-\infty, 0]$ on $[0, 1]$, and $\cos(\log(x))$ generates and infinite number of oscillations as a result. The integrand is like a cosine wave with a frequency that is infinite at $x=0$, and which decreases as $x$ increases. The integral has the same sort of infinitely
oscillatory behavior, but the amplitude of the oscillations is zero at x=0 and grows with x.

iv. Numerically, find two distinct roots of the integral and the integrand for x > 0.

More than 2 roots are found here as an example. Because the integrand and integral are oscillatory in nature, there are infinitely many distinct roots, and not all are real.

```
FindRoot[integrand, {x, 0.000001}]
FindRoot[integrand, {x, 0.001}]
FindRoot[integrand, {x, 0.01}]
FindRoot[integrand, {x, 0.1}]
FindRoot[integrand, {x, 0.5}]
FindRoot[integrand, {x, 2}]
FindRoot[integrand, {x, 24}]
FindRoot[integrand, {x, 25}]
{x -> 7.24947 \times 10^{-7} }
{x -> 0.000388203 }
{x -> 0.00898329}
{x -> 0.20788}
{x -> 0.20788}
{x -> 4.81048}
{x -> 4.81048}
{x -> 111.318}
FindRoot[integral, {x, 0.000001}]
FindRoot[integral, {x, 0.0001}]
FindRoot[integral, {x, 0.01}]
FindRoot[integral, {x, 0.1}]
FindRoot[integral, {x, 0.5}]
FindRoot[integral, {x, 2}]
FindRoot[integral, {x, 24}]
FindRoot[integral, {x, 25}]
{x -> 1.59002 \times 10^{6} }
{x -> 0.000036794 }
{x -> 0.197029}
{x -> 0.000851438 + 3.446 \times 10^{-17} i}
{x -> 0.455938}
{x -> 0.197029}
{x -> 10.5507}
{x -> 10.5507}
```

Individual Exercise I2-4 (50 points)

Write a function that takes a list of numbers as an argument and returns 5 numbers: the length of the list and its average, standard deviation, maximum, and minimum. Your function should work for a list of arbitrary length. Demonstrate that your function works.
The desired function could be constructed as follows:

```math
listAnalyzer[list_] :=
{Length[list], Mean[list], StandardDeviation[list], Max[list], Min[list];
```

To demonstrate that the function works, data with a known standard deviation and mean will be used. The NormalDistribution function produces a bell curve with mean zero and standard deviation 1. Here, random points are selected, but their selection is weighted by the normal distribution. As more points are selected, the mean and standard deviation of the random normally-distributed arrays can be seen to approach 0 and 1, respectively.

```math
analyzerTester = Table[listAnalyzer[RandomReal[NormalDistribution[], 10^i]], {i, 8}]
```

Show[ListPlot[Table[analyzerTester[[i, 2]], {i, 8}], AxesLabel -> {Style["Log[length of list]", FontSize -> 18], Style["mean value", FontSize -> 18]}, PlotStyle -> {PointSize[Large], Blue}],
```
The above plots show that as the number of points grows, the mean and standard deviation stabilize to the expected values.

To demonstrate that the max & min portions of listAnalyzer are working as expected, we know that as more points are sampled randomly from the normal distribution, more extreme values will be found. In the limit of infinitely many points in the list, 68.2% of them will be within 1 standard deviation from the mean, 27.2% of the points will have $1 \leq |x| \leq 2$, and 4.2% of the points will be in $2 \leq |x| \leq 3$. Only about 3 in 1000 points will have an absolute value greater than 3, and the odds continue to decrease the further the value is from zero. Looking at the max and min members of the list as a function of list length, more and more “rare” points occur as the list gets loner.

```mathematica
ListPlot[{Table[analyzerTester[[i, 4]], {i, 8}], Table[analyzerTester[[i, 5]], {i, 8}]}, AxesLabel -> {Style["Log[length of list]", FontSize -> 18], Style["max & min members of the list", FontSize -> 18]}, PlotRange -> All, PlotStyle -> {{PointSize[Large], Orange}, {PointSize[Large], Purple}}, PlotMarkers -> Automatic]
```

max & min members of the list

![Graph showing max & min members of the list](image)

Individual Exercise I2-5 (50 points)

### i. For the following Mathematica code snippets, display its result and, using one or two sentences, explain how that result follows from the code.

```mathematica
j = 1;
Table[j++, {i, 1, 20}]
j
```

{1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20}

21

```mathematica
i = 100;
Table[i++, {i, 1, 20}]
i
```

{1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 20}

100

In both cases, the increment function `x++` does the following: increase the value of `x` by 1, and return the old value of `x`. This is why the first step in each case returns 1, not 2.

In the first case, `j` is *not* a dummy variable/ the iterator, so the operation `j++` is conducted on the actual value of `j`.
times. This causes the value of j to be 21 after the operation.

In the second case, the iterator “i” is a dummy variable that is defined within Table, so changing it has no affect on the value of “i” stored outside the Table function, thus “i” (outside) still equals 100. Only the iterator “i” experiences the increases due to repeated ++ing. Also, “i” (iterator) gets redefined each step, so the ++ isn’t actually affecting anything.

ii. For the following three Mathematica code snippets, display their results and explain why their results differ.

- a
  ```mathematica
  fOne[i] = {i,DateString[]}
  Table[Pause[1]; fOne[j], {j, 1, 5}]
  {100, Wed 19 Sep 2012 11:54:07}
  {fOne[1], fOne[2], fOne[3], fOne[4], fOne[5]}
  ```
  This is a simple definition for fOne[i]. There is no function “fOne”, just the variable “fOne[i]”. “fOnes[1]” however is not defined, so Mathematica just returns variable names without any computation, as they are unassigned.

- b
  ```mathematica
  fTwo[i_] = {i,DateString[]}
  Table[Pause[1]; fTwo[j], {j, 1, 5}]
  {100, Wed 19 Sep 2012 11:54:23}
  {{1, Wed 19 Sep 2012 11:54:23},
   {2, Wed 19 Sep 2012 11:54:23},
   {3, Wed 19 Sep 2012 11:54:23},
   {4, Wed 19 Sep 2012 11:54:23},
   {5, Wed 19 Sep 2012 11:54:23}}
  ```
  The variable “i” was defined in the previous problem, so it simply prints the value of “i” with the DataString at the time fTwo[i] is first evaluated. This definition is set “=”, not set-delayed “:=”, so it does not recompute the assignment each time.
  
  If you cleared the vale of “i”, the result is instead:
  ```mathematica
  Clear[i]
  fTwo[i_] = {i,DateString[]}
  Table[Pause[1]; fTwo[j], {j, 1, 5}]
  {i, Wed 19 Sep 2012 11:59:53}
  {{1, Wed 19 Sep 2012 11:59:53},
   {2, Wed 19 Sep 2012 11:59:53},
   {3, Wed 19 Sep 2012 11:59:53},
   {4, Wed 19 Sep 2012 11:59:53},
   {5, Wed 19 Sep 2012 11:59:53}}
  ```
  Again, the value of “i” is simply passed into the placeholder position in fTwo[i], however, DateString is not re-evaluated because this definition is set “=”, not set-delayed “:=”.

- c
  ```mathematica
  fThree[i_] := {i,DateString[]}
  Table[Pause[1]; fThree[j], {j, 1, 5}]
  {{1, Wed 19 Sep 2012 11:54:35},
   {2, Wed 19 Sep 2012 11:54:36},
   {3, Wed 19 Sep 2012 11:54:37},
   {4, Wed 19 Sep 2012 11:54:38},
   {5, Wed 19 Sep 2012 11:54:39}}
  ```
  The use of “i_” causes i to be a placeholder in the function fThree[i], and the set-delayed “:=” forces the whole function to recompute every time “fThree” is called.

Individual Exercise I2-6 (10 points)
i. Find the eigenvalues and eigenvectors of the matrix

\[
\begin{pmatrix}
    a & b + i c \\
    b - i c & d
\end{pmatrix}
\]

To find eigenvalues and eigenvectors simultaneously, use Eigensystem:

\[
\text{eigenAnswer} = \text{Eigensystem}[\{(a, b + i c), \{b - i c, d\}\}]
\]

\[
\left\{ \left\{ \frac{1}{2} \left( a + d - \sqrt{a^2 + 4 b^2 + 4 c^2 - 2 a d + d^2} \right), \frac{1}{2} \left( a + d + \sqrt{a^2 + 4 b^2 + 4 c^2 - 2 a d + d^2} \right) \right\}, \left\{ \frac{-a + d + \sqrt{a^2 + 4 b^2 + 4 c^2 - 2 a d + d^2}}{2 (b - i c)}, 1 \right\} \right\}
\]

The first element of the list eigenAnswer is a list of the eigenvalues, and the second element is a list of corresponding eigenvectors.

\[
\text{eigValues} = \text{eigenAnswer}[[1]]
\]

\[
\left\{ \frac{1}{2} \left( a + d - \sqrt{a^2 + 4 b^2 + 4 c^2 - 2 a d + d^2} \right), \frac{1}{2} \left( a + d + \sqrt{a^2 + 4 b^2 + 4 c^2 - 2 a d + d^2} \right) \right\}
\]

\[
\text{eigVectors} = \text{eigenAnswer}[[2]]
\]

\[
\left\{ \frac{-a + d + \sqrt{a^2 + 4 b^2 + 4 c^2 - 2 a d + d^2}}{2 (b - i c)}, 1 \right\}, \left\{ \frac{-a + d - \sqrt{a^2 + 4 b^2 + 4 c^2 - 2 a d + d^2}}{2 (b - i c)}, 1 \right\}
\]

ii. If a, b, c, and d are real numbers, what condition(s) must be fulfilled such that all the eigenvalues are real?

For the eigenvalues \( \frac{1}{2} \left( a + d \pm \sqrt{a^2 + 4 b^2 + 4 c^2 - 2 a d + d^2} \right) \) to be real, the value inside the square root must be non-negative. To test this with Mathematica, use Reduce, and specify that the domain for \{a, b, c, d\} is the real number line:

\[
\text{Reduce}[a^2 + 4 b^2 + 4 c^2 - 2 a d + d^2 \geq 0, \{a, b, c, d\}, \text{Reals}]
\]

True

This result means that the item inside the square root is always non-negative, regardless of the values of a and d. All matrices of this form will have real eigenvalues. It turns out that there are many physical situations in which having real eigenvalues is important. Such matrices are called “Hermitian.”

Indiviuall Exercise I2-7 (20 points)

Find the solution to the Shrodinger equation for a particle in a parabolic well centered at the origin:

\[
\frac{-h^2}{2m} \frac{d^2 \Psi}{dx^2} + k x^2 \Psi = E \Psi
\]
The first function that comes to mind to aid in solving an equation is “Solve.” However, this is not an ordinary algebraic equation. It is a differential equation, so the function “DSolve” is appropriate here.

\[
\text{wavefxn} = \text{DSolve}\left[\left\{\left(-\frac{h^2}{2m}\right) \psi''[x] + k x^2 \psi[x] = \text{Etot} \psi[x]\right\}, \psi[x], x\right]\]

\[
\left\{\psi[x] \rightarrow C[2] \text{ParabolicCylinderD}\left[\frac{-\sqrt{2} \text{Etot} \sqrt{m} - \sqrt{k} \frac{2^{3/4} k^{1/4} m^{1/4} x}{h}}{2^{3/4} k^{1/4} m^{1/4} x} + \frac{\sqrt{2} \text{Etot} \sqrt{m} - \sqrt{k} \frac{2^{3/4} k^{1/4} m^{1/4} x}{h}}{2^{3/4} k^{1/4} m^{1/4} x}\right]\right\}
\]

The result is an unfamiliar, but it is a perfectly good answer: the function \(\psi[x]\) is given in a closed form.

**Individual Exercise I2-8 (90 points)**

The critical point occurs at the temperature for which an inflection point, a maximum, and a minimum appear at same \(\bar{V}\) in the \(P = f_P(\bar{V}, T = \text{const})\) isotherm plot. The critical point condition is equivalent to the condition that \(\partial f_P/\partial V = 0\) and \(\partial^2 f_P/\partial V^2 = 0\) (why?).

The critical point occurs at a saddle point. A saddle point is a point that is a stationary point \(f'=0\), but not a maximum or minimum (which can only be satisfied if \(f''=0\)). An example of a function that contains a saddle point is \(f(x) = x^3\) at \(x = 0\), \(f' = 0\) and \(f'' = 0\).

\[
\text{Plot}\left[\text{PlotLabel} \rightarrow \text{Style}["Example of a saddle point: } x^3|x=0", \text{FontSize} \rightarrow 20]\right]
\]

Example of a saddle point: \(x^3 | x=0\)

---

**i. Find the critical point temperature \(T_{crit}, P_{crit}, \text{and } \bar{V}_{crit}\).**

To find the critical point of \(f_P\), simultaneously solve \(\partial P/\partial V = 0\) and \(\partial^2 P/\partial V^2 = 0\):

\[
\text{criticalTandV} = \text{Solve}\left[\left\{\text{dPdV} = 0, \text{D}[\text{dPdV}, \text{molarV}] = 0\right\}, \{\text{molarV}, T\}\right][[1]]
\]

\[
\left\{\text{molarV} \rightarrow 3 \text{ b}, T \rightarrow -\frac{8 a}{27 \text{ b R}}\right\}
\]
The critical point pressure is found by substituting \( T_{\text{crit}} \) and \( V_{\text{crit}} \) back into \( f_P \).

\[
P_{\text{crit}} = \frac{\text{vdwP}}{(T \to T_{\text{crit}}, \text{molarV} \to V_{\text{crit}})}
\]

\[
a - \frac{9}{27 b^2}
\]

Note that the van der Waals equation, \( \partial P/\partial V = 0 \), and \( \partial^2 P/\partial V^2 = 0 \) together makes three equations. \( P_{\text{crit}}, V_{\text{crit}}, T_{\text{crit}}, a, \) and \( b \) makes 5 unknowns. The system can only be reduced to 2 unknowns (not completely solved) because 5 equations minus 3 unknowns = 2 remaining unknowns. Therefore, any 3 of the unknowns can be written in terms of the other 2 unknowns. Here, we have \( T_{\text{crit}}, P_{\text{crit}}, \) and \( V_{\text{crit}} \) in terms of \( a \) and \( b \).

### ii. Calculate \( a \) and \( b \) in terms of \( T_{\text{crit}} \) and \( V_{\text{crit}} \).

Above, we have \( T_{\text{crit}} \) and \( V_{\text{crit}} \) in terms of \( a \) and \( b \). Rearranging the equations yields \( a \) and \( b \) in terms of \( T_{\text{crit}} \) and \( V_{\text{crit}} \).

\[
\text{criticalAandB} = \text{Solve}([Tc = T_{\text{crit}}, Vc = V_{\text{crit}}], \{a, b\})[[1]]
\]

\[
\{a \to \frac{9 - R T_{\text{crit}} V_{\text{crit}}}{8}, b \to \frac{V_{\text{crit}}}{3}\}
\]

\[
A_{\text{crit}} = a / . \text{criticalAandB}
\]

\[
B_{\text{crit}} = b / . \text{criticalAandB}
\]

\[
a = \frac{9 - R T_{\text{crit}} V_{\text{crit}}}{8}
\]

\[
b = \frac{V_{\text{crit}}}{3}
\]

Note that because \( T_{\text{crit}} \) and \( V_{\text{crit}} \) are defined above in terms of \( a \) and \( b \), new symbols are required (\( T_c \) and \( V_c \)) to act as the symbols for \( T_{\text{critical}} \) and \( V_{\text{critical}} \).

### iii. Replace \( a \) and \( b \) in the van der Waals equation and find the relation between \( T_{\text{crit}}, P_{\text{crit}}, \) and \( \overline{V}_{\text{crit}} \).

The critical pressure occurs where \( a, b, T, \) and \( \overline{V} \) take their resective critical point values.

\[
P_c = \frac{\text{vdwP}}{(a \to A_{\text{crit}}, b \to B_{\text{crit}}, T \to T_{\text{crit}}, \text{molarV} \to V_{\text{crit}})}
\]

\[
P_c = \frac{3 R T_{\text{crit}}}{8 V_{\text{crit}}}
\]

Above is the relationship between the critical values of pressure, temperature, and molar volume. If we rearrange it, it looks like:

\[
P_c \overline{V}_{c} = \frac{3 R}{8} T_{c}
\]

This looks exactly like the ideal gas law, but with a factor of 3/8. However, it is not like the ideal gas law because none of the values are free variables: \( P_c, \overline{V}_{c}, \) and \( T_c \) are all material properties.