Chapter 2

Mathematical Functions

EXERCISES

Exercise 2.1. Enter a formula into cell $D2$ that will compute the mean of the numbers in cells $A2, B2$, and $C2$.

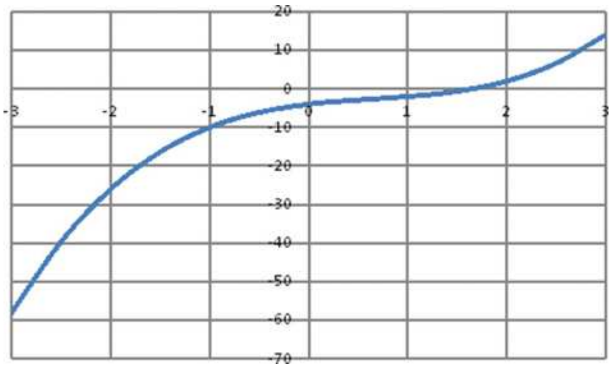
$$= (A2 + B2 + C2)/3$$

Exercise 2.2. Construct a graph representing the function

$$y(x) = x^3 - 2x^2 + 3x + 4 \tag{2.1}$$

Use Excel or Mathematica or some other software to construct your graph.

Here is the graph, constructed with Excel:



Exercise 2.3. Generate the negative logarithms in the short table of common logarithms.

x	$y = \log_{10}(x)$	x	$y = \log_{10}(x)$
1	0	0.1	−1
10	1	0.01	−2
100	2	0.001	−3
1000	3	0.0001	−4

$$0.1 = 1/10$$

$$\log(0.1) = -\log(10) = -1$$

$$0.01 = 1/100$$

$$\log(0.01) = -\log(100) = -2$$

$$0.001 = 1/1000$$

$$\log(0.001) = -\log(1000) = -3$$

$$0.0001 = 1/10000$$

$$\log(0.001) = -\log(10000) = -4$$

Exercise 2.4. Using a calculator or a spreadsheet, evaluate the quantity $(1 + \frac{1}{n})^n$ for several integral values of n ranging from 1 to 1,000,000. Notice how the value approaches the value of e as n increases and determine the value of n needed to provide four significant digits.

Here is a table of values

x	$(1 + 1/n)^n$
1	2
2	2.25
5	2.48832
10	2.59374246
100	2.704813829
1000	2.716923932
10000	2.718145927
100000	2.718268237
1000000	2.718280469

Mathematics for Physical Chemistry. http://dx.doi.org/10.1016/B978-0-12-415809-2.00026-4

To twelve significant digits, the value of e is 2.71828182846. The value for $n = 1000000$ is accurate to six significant digits. Four significant digits are obtained with $n = 10000$.

Exercise 2.5. Without using a calculator or a table of logarithms, find the following:

a. $\ln(100.000) = \ln(10)\log_{10}(100.000)$
$= (2.30258509\cdots)(2.0000) = 4.60517$

b. $\ln(0.0010000) = \ln(10)\log_{10}(0.0010000)$
$= (2.30258509\cdots)(-3.0000) = -6.90776$

c. $\log_{10}(e) = \dfrac{\ln(e)}{\ln(10)} = \dfrac{1}{2.30258509\cdots} = 0.43429\cdots$

Exercise 2.6. For a positive value of b find an expression in terms of b for the change in x required for the function e^{bx} to double in size.

$$\frac{f(x+\Delta x)}{f(x)} = 2 = \frac{e^{b(x+\Delta x)}}{e^{bx}} = e^{b\Delta x}$$

$$\Delta x = \frac{\ln(2)}{b} = \frac{0.69315\cdots}{b}$$

Exercise 2.7. A reactant in a first-order chemical reaction without back reaction has a concentration governed by the same formula as radioactive decay,

$$[\mathrm{A}]_t = [\mathrm{A}]_0 e^{-kt},$$

where $[\mathrm{A}]_0$ is the concentration at time $t = 0$, $[\mathrm{A}]_t$ is the concentration at time t, and k is a function of temperature called the rate constant. If $k = 0.123\ \mathrm{s}^{-1}$ find the time required for the concentration to drop to 21.0% of its initial value.

$$t = \left(\frac{1}{k}\right)\ln\left(\frac{[\mathrm{A}]_0}{[\mathrm{A}]_t}\right) = \left(\frac{1}{0.123\ \mathrm{s}^{-1}}\right)\ln\left(\frac{100.0}{21.0}\right)$$
$$= 12.7\ \mathrm{s}$$

Exercise 2.8. Using a calculator, find the value of the cosine of 15.5° and the value of the cosine of 375.5°. Display as many digits as your calculator is able to display. Check to see if your calculator produces any round-off error in the last digit. Choose another pair of angles that differ by 360° and repeat the calculation. Set your calculator to use angles measured in radians. Find the value of sin (0.3000). Find the value of sin $(0.3000 + 2\pi)$. See if there is any round-off error in the last digit.

$$\begin{aligned}
\cos(15.5^\circ) &= 0.96363045321 \\
\cos(375.5^\circ) &= 0.96363045321 \\
\sin(0.3000) &= 0.29552020666 \\
\sin(0.3000 + 2\pi) &= \sin(6.58318530718) \\
&= 0.29552020666
\end{aligned}$$

There is no round-off error to 11 digits in the calculator that was used.

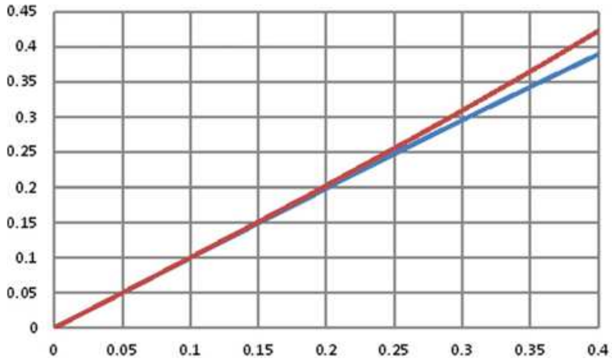
Exercise 2.9. Using a calculator and displaying as many digits as possible, find the values of the sine and cosine of 49.500°. Square the two values and add the results. See if there is any round-off error in your calculator.

$$\sin(49.500^\circ) = 0.7604059656$$

$$\cos(49.500^\circ) = 0.64944804833$$

$$(0.7604059656)^2 + (0.64944804833)^2 = 1.00000000000$$

Exercise 2.10. Construct an accurate graph of $\sin(x)$ and $\tan(x)$ on the same graph for values of x from 0 to 0.4 rad and find the maximum value of x for which the two functions differ by less than 1%.



The two functions differ by less than 1% at 0.14 rad. Notice that at 0.4 rad, $\sin(x) \prec x \prec \tan(x)$ and that the three quantities differ by less than 10%.

Exercise 2.11. For an angle that is nearly as large as $\pi/2$, find an approximate equality similar to Eq. (2.36) involving $(\pi/2) - \alpha$, $\cos(\alpha)$, and $\cot(\alpha)$.

Construct a right triangle with angle with the angle $(\pi/2) - \alpha$, where α is small. The triangle is tall, with a small value of x (the horizontal leg) and a larger value of y (the vertical leg). Let r be the hypotenuse, which is nearly equal to y.

$$\cos((\pi/2) - \alpha) = \frac{x}{r}$$

$\cot((\pi/2) - \alpha) = \frac{x}{y} \approx \frac{x}{r}$. The measure of the angle in radians is equal to the arc length subtending the angle α divided by r and is very nearly equal to x/r. Therefore

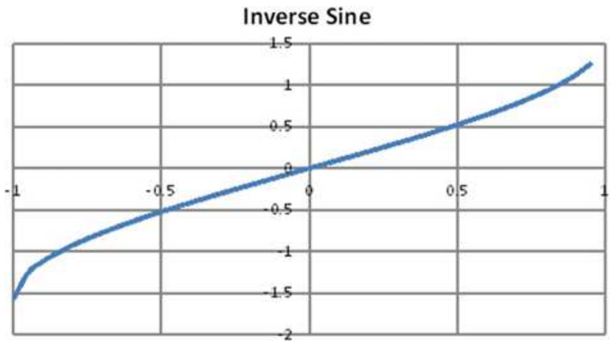
$$\cos((\pi/2) - \alpha) \approx \alpha$$

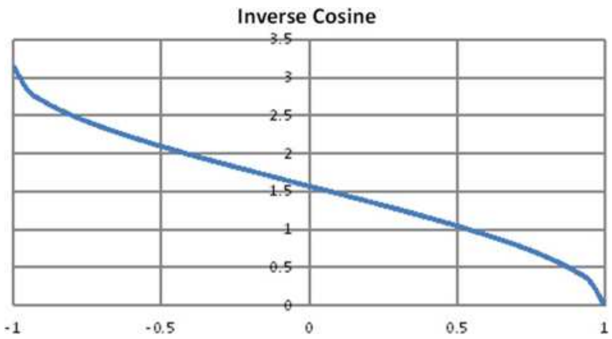
$$\cot((\pi/2) - \alpha) \approx \alpha$$

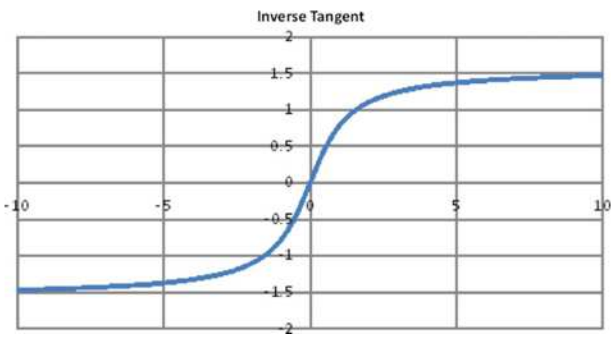
$$\cos((\pi/2) - \alpha) \approx \cot((\pi/2) - \alpha)$$

Exercise 2.12. Sketch graphs of the arcsine function, the arccosine function, and the arctangent function. Include only the principal values.

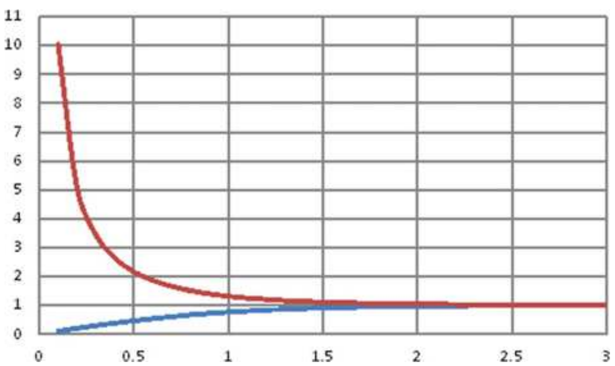
Here are accurate graphs:







Exercise 2.13. Make a graph of $\tanh(x)$ and $\coth(x)$ on the same graph for values of x ranging from 0.1 to 3.0.



Exercise 2.14. Determine the number of significant digits in $\sin(95.5°)$.

We calculate $\sin(95.45°)$ and $\sin(95.45°)$. Using a calculator that displays 8 digits, we obtain

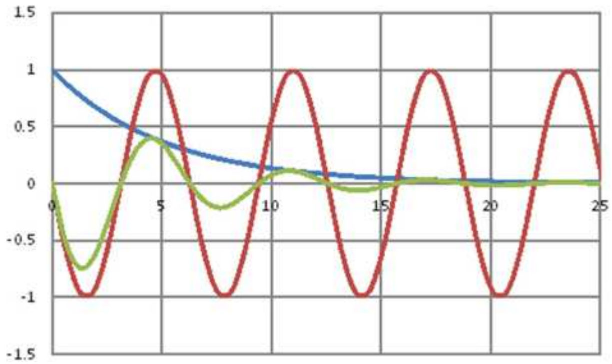
$$\sin(95.45°) = 0.99547946$$

$$\sin(95.55°) = 0.99531218$$

We report the sine of 95.5° as 0.9954, specifying four significant digits, although the argument of the sine was given with three significant digits. We have followed the common policy of reporting a digit as significant if it might be incorrect by one unit.

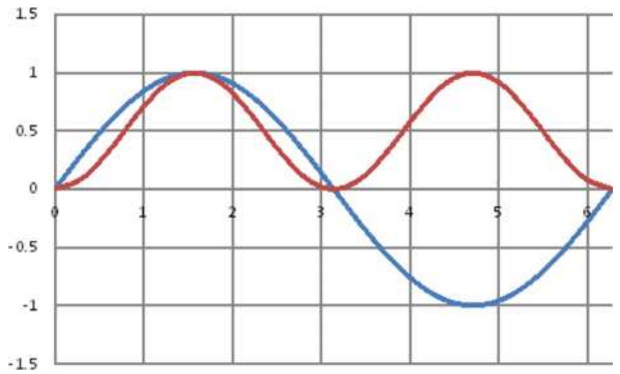
Exercise 2.15. Sketch rough graphs of the following functions. Verify your graphs using Excel or Mathematica.

a. $e^{-x/5}\sin(x)$. Following is a graph representing each of the factors and their product:



b. $\sin^2(x) = [\sin(x)]^2$

Following is a graph representing $\sin(x)$ and $\sin^2(x)$.



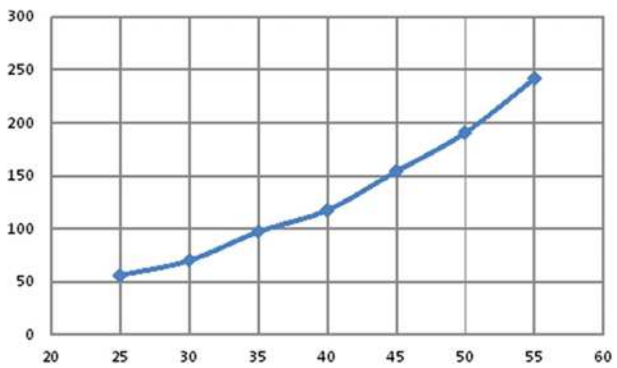
PROBLEMS

1. The following is a set of data for the vapor pressure of ethanol taken by a physical chemistry student. Plot these points by hand on graph paper, with the temperature on the horizontal axis (the abscissa) and

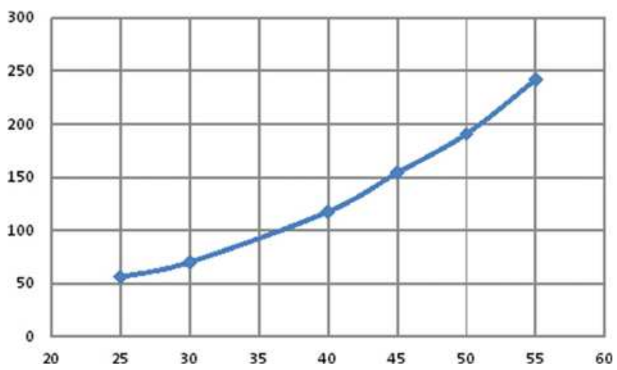
the vapor pressure on the vertical axis (the ordinate). Decide if there are any bad data points. Draw a smooth curve nearly through the points, disregarding any bad points. Use Excel to construct another graph and notice how much work the spreadsheet saves you.

Temperature/°C	Vapor pressure/torr
25.00	55.9
30.00	70.0
35.00	97.0
40.00	117.5
45.00	154.1
50.00	190.7
55.00	241.9

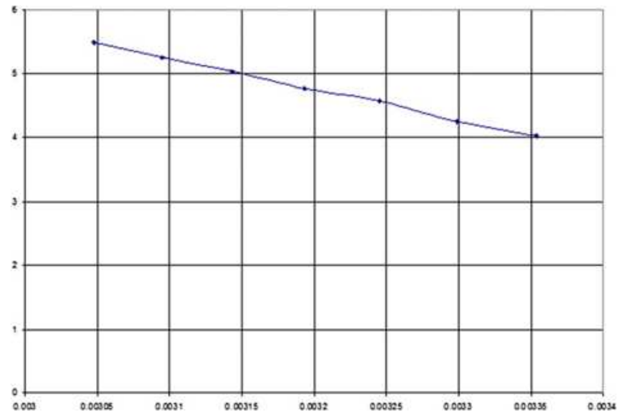
Here is a graph constructed with Excel:



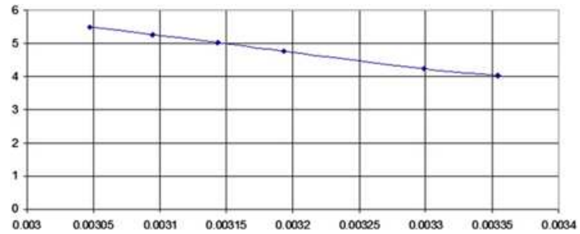
The third data point might be suspect. Here is a graph omitting that data point:



2. Using the data from the previous problem, construct a graph of the natural logarithm of the vapor pressure as a function of the reciprocal of the Kelvin temperature. Why might this graph be more useful than the graph in the previous problem?



This graph might be more useful than the first graph because the function is nearly linear. However, the third data point still lies off the curve. Here is a graph with that data point omitted.



Thermodynamic theory implies that it should be nearly linear if there were no experimental error.

3. A reactant in a first-order chemical reaction without back reaction has a concentration governed by the same formula as radioactive decay,

$$[\mathrm{A}]_t = [\mathrm{A}]_0 e^{-kt},$$

where $[\mathrm{A}]_0$ is the concentration at time $t = 0$, $[\mathrm{A}]_t$ is the concentration at time t, and k is a function of temperature called the rate constant. If $k = 0.232\ \mathrm{s}^{-1}$ at 298.15 K find the time required for the concentration to drop to 33.3% of its initial value at a constant temperature of 298.15 K.

$$t = \frac{\ln\left([\mathrm{A}]_0/[\mathrm{A}]_t\right)}{k} = \frac{\ln(1/0.333)}{0.232\ \mathrm{s}^{-1}} = 4.74\ \mathrm{s}$$

4. Find the value of each of the hyperbolic trigonometric functions for $x = 0$ and $x = \pi/2$. Compare these values with the values of the ordinary (circular) trigonometric functions for the same values of the independent variable.

Here are two table of values:

x	sinh(x)	cosh(x)	tanh(x)	csch(x)	sech(x)	coth(x)
0	0	1	0	∞	1	∞
$\pi/2$	2.3013	2.5092	0.91715	0.43454	0.39854	1.09033

x	sin(x)	cos(x)	tan(x)	csc(x)	sec(x)	cot(x)
0	0	1	0	∞	0	∞
$\pi/2$	1	0	∞	1	∞	0

5. Express the following with the correct number of significant digits. Use the arguments in radians:

a. tan (0.600)

$$\tan(0.600) = 0.684137$$
$$\tan(0.5995) = 0.683403$$
$$\tan(0.60005) = 0.684210$$

We report $\tan(0.600) = 0.684$. If a digit is probably incorrect by 1, we still treat it as significant.

b. sin (0.100)

$$\sin(0.100) = 0.099833$$
$$\sin(0.1005) = 0.100331$$
$$\sin(0.0995) = 0.099336$$

We report $\sin(0.100) = 0.100$.

c. cosh (12.0)

$$\cosh(12.0) = 81377$$
$$\cosh(12.05) = 85550$$
$$\cosh(11.95) = 77409$$

We report $\cosh(12.0) = 8 \times 10^4$. There is only one significant digit.

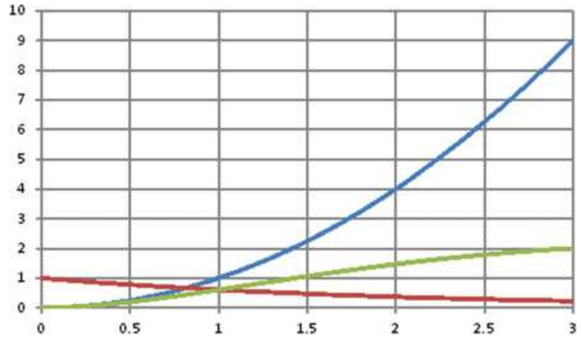
d. sinh (10.0)

$$\sinh(10.0) = 11013$$
$$\sinh(10.01) = 11578$$
$$\sinh(9.995) = 10476$$

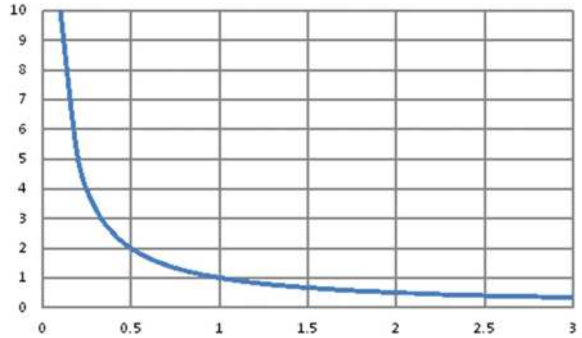
We report $\sinh(10.0) = 11000 = 1.1 \times 10^4$

6. Sketch rough graphs of the following functions. Verify your graphs using Excel or Mathematica:

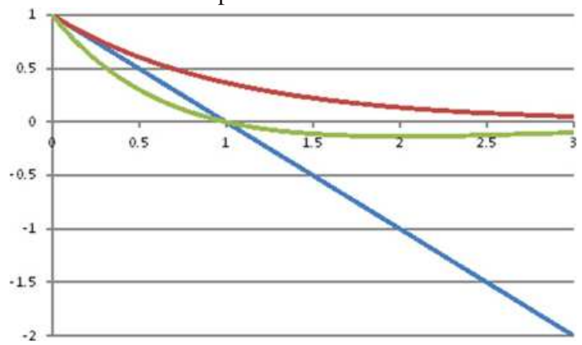
a. $x^2e^{-x/2}$ Following is a graph of the two factors and their product.



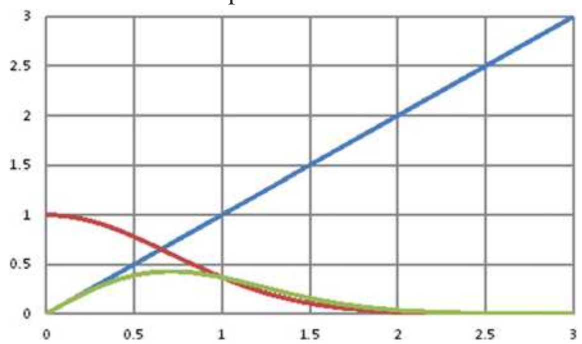
b. $1/x^2$ Following is the graph:



c. $(1-x)e^{-x}$ Following is a graph showing each factor and their product.



d. xe^{-x^2} Following is a graph showing the two factors and their product.



7. Tell where each of the following functions is discontinuous. Specify the type of discontinuity:

a. $\tan(x)$ Infinite discontinuities at $x = \pi/2$, $x = 3\pi/2$, $x = 5\pi/2, \cdots$
b. $\csc(x)$ Infinite discontinuities at $x = 0$, $x = \pi$, $x = 2\pi, \cdots$
c. $|x|$ Continuous everywhere, although there is a sharp change of direction at $x = 0$.

8. Tell where each of the following functions is discontinuous. Specify the type of discontinuity:

a. $\cot(x)$ Infinite discontinuities at $x = 0, x = \pi$, $x = 2\pi, \cdots$
b. $\sec(x)$ Infinite discontinuities at $x = \pi/2$, $x = 3\pi/2$, $x = 5\pi/2, \cdots$
c. $\ln(x-1)$ Infinite discontinuity at $x = 1$, function not defined for $x \prec 1$.

9. If the two ends of a completely flexible chain (one that requires no force to bend it) are suspended at the same height near the surface of the earth, the curve representing the shape of the chain is called a catenary. It can be shown[1] that the catenary is represented by

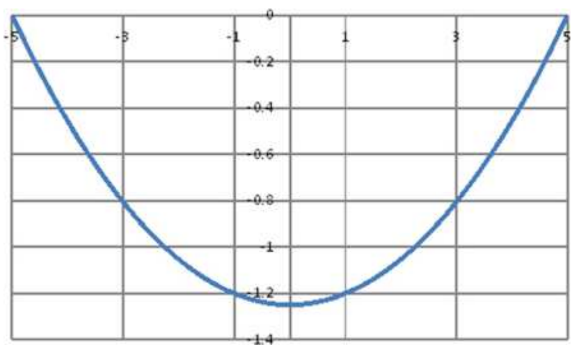
$$y = a\cosh\left(\frac{x}{a}\right)$$

where

$$a = \frac{T}{g\rho}$$

and where ρ is the mass per unit length, g is the acceleration due to gravity, and T is the tension force on the chain. The variable x is equal to zero at the center of the chain. Construct a graph of this function such that the distance between the two points of support is 10.0 m and the mass per unit length is 0.500 kg m^{-1}, and the tension force is 50.0 N.

$$a = \frac{T}{g\rho} = \frac{50.0 \text{ kg m s}^2}{(9.80 \text{ m}^2 \text{ s}^{-2})(0.500 \text{ kg m}^{-1})} = 10.20 \text{ m}$$
$$y = (10.20 \text{ m})\cosh(x/10.20 \text{ m})$$



[1] G. Polya, Mathematical Methods in Science, The Mathematical Association of America, 1977, pp. 178ff.

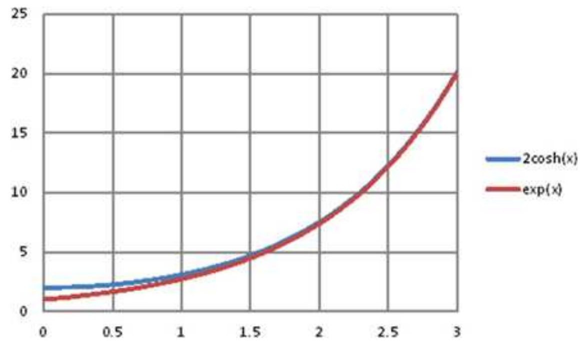
For this graph, we have plotted $y - 11.4538$ such that this quantity vanishes at the ends of the chain.

10. For the chain in the previous problem, find the force necessary so that the center of the chain is no more than 0.500 m lower than the ends of the chain.

By trial and error, we found that the center of the chain is 0.499 m below the ends when $a = 25.5$ m. This corresponds to

$$T = g\rho a = (9.80 \text{ m s}^{-2})(0.500 \text{ kg m}^{-1})(25.5 \text{ m}) = 125 \text{ N}$$

11. Construct a graph of the two functions: $2\cosh(x)$ and e^x for values of x from 0 to 3. At what minimum value of x do the two functions differ by less than 1%?



By inspection in a column of values of the difference, the two functions differ by less than 1% at $x = 2.4$.

12. Verify the trigonometric identity

$$\sin(x+y) = \sin(x)\cos(y) + \cos(x)\sin(y)$$

for the angles $x = 1.00000$ rad, $y = 2.00000$ rad. Use as many digits as your calculator will display and check for round-off error.

$$\sin(3.00000) = 0.14112000806$$
$$\sin(1.00000)\cos(2.00000) + \cos(1.00000) \times \sin(2.00000) = 0.14112000806$$

There was no round-off error in the calculator that was used.

13. Verify the trigonometric identity

$$\cos(2x) = 1 - 2\sin^2(x)$$

for $x = 0.50000$ rad. Use as many digits as your calculator will display and check for round-off error.

$$\cos(1.00000) = 0.54030230587$$
$$1 - 2\sin^2(0.50000) = 1 - 0.45969769413 = 0.54030230587$$

There was no round-off error to 11 significant digits in the calculator that was used.