

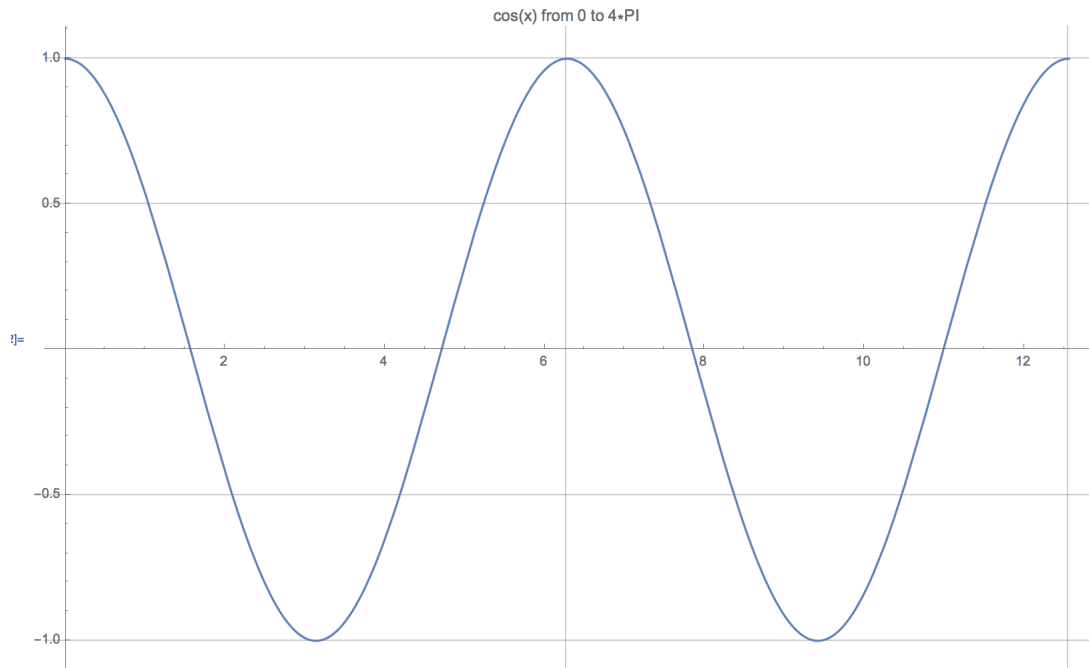
# Chem/Stat3240: Homework 1b

## Mathematica

August 31, 2016

- 4 Write the code that takes real numbers  $L$  and  $R$  and determines the maximum value of  $f(x) = \cos(x)$  on the interval  $[L, R]$ . Assume  $L < R$ . Recall that the cosine achieves a maximum value of 1 at integral multiples of  $2\pi$ . The intention of the problem is to use a conditional to determine if the interval contains a multiple of  $2\pi$ . If so, cosine is equal to 1 somewhere on the interval. Otherwise, one of the interval endpoints is the maximum. Useful commands for this problem are `Floor`, `Ceiling`, and `Max`. See the plot below for insight into how to construct the test.

Submit your code as a function in the file `intervalMax.nb` and the tests in the .zip to the collab site.



5 For large  $n$ ,

$$R_n = 1 - \frac{1}{3} + \cdots + \frac{(-1)^{n+1}}{2n-1} = \sum_{k=1}^n \frac{(-1)^{k+1}}{2k-1} \approx \frac{\pi}{4}$$

$$T_n = 1 + \frac{1}{2^2} + \cdots + \frac{1}{n^2} = \sum_{k=1}^n \frac{1}{k^2} \approx \frac{\pi^2}{6}$$

$$U_n = 1 + \frac{1}{2^4} + \cdots + \frac{1}{n^4} = \sum_{k=1}^n \frac{1}{k^4} \approx \frac{\pi^4}{90}$$

giving two different ways to estimate  $\pi$ :

$$\begin{aligned} \rho_n &= 4R_n \\ \tau_n &= \sqrt{6T_n} \\ \mu_n &= (90U_n)^{1/4} \end{aligned}$$

For a given value of  $n$ , write the code to compute the estimates  $\rho_n$ ,  $\tau_n$ , and  $\mu_n$  in the body of the function template `piEst1` and run the test suite until it passes the tests.

Now write a script `hwk2_1.nb` that uses the code for your estimates (without the function wrapper) and displays the value of  $|\pi - \rho_n|$ ,  $|\pi - \tau_n|$ , and  $|\pi - \mu_n|$  for  $n = 100, 200, 300, \dots, 1000$ . Remember to initialize variables to store partial sums. You should also be able to use one `Do` loop and avoid recomputing previous partial sums, instead of separate loops for each partial sum. Useful commands are `Do`, `Abs`, `Mod`, `Sqrt`, and `Power`.

Format the output as a 3-column table with the first column being values of  $n$ , and appropriate headers for each column as shown below.

Commands you will find useful in formatting the output are `PaddedForm` for the first column and `ScientificForm` for the subsequent columns. It is also useful to specify the degree of precision with the `N` command.

```
= << hwk2_1.m
```

n	R_error	T_error	U_error
100	$9.99975 \times 10^{-3}$	$9.51612 \times 10^{-3}$	$2.38282 \times 10^{-7}$
200	$4.99997 \times 10^{-3}$	$4.76635 \times 10^{-3}$	$3.00098 \times 10^{-8}$
300	$3.33332 \times 10^{-3}$	$3.17941 \times 10^{-3}$	$8.91407 \times 10^{-9}$
400	$2.50000 \times 10^{-3}$	$2.38525 \times 10^{-3}$	$3.76533 \times 10^{-9}$
500	$2.00000 \times 10^{-3}$	$1.90853 \times 10^{-3}$	$1.92929 \times 10^{-9}$
600	$1.66667 \times 10^{-3}$	$1.59063 \times 10^{-3}$	$1.11705 \times 10^{-9}$
700	$1.42857 \times 10^{-3}$	$1.36351 \times 10^{-3}$	$7.03699 \times 10^{-10}$
800	$1.25000 \times 10^{-3}$	$1.19314 \times 10^{-3}$	$4.71550 \times 10^{-10}$
900	$1.11111 \times 10^{-3}$	$1.06062 \times 10^{-3}$	$3.31253 \times 10^{-10}$
1000	$1.00000 \times 10^{-3}$	$9.54597 \times 10^{-4}$	$2.41524 \times 10^{-10}$

Submit `piEst1.nb`, the script `hwk2_1.nb`, and the test suite in the `.zip` file to the collab site.

**Remember to comment your code as shown in the example below**

```

In[11]:= sphereArea[r_] :=
(* sphereArea(r):Calculates the surface area of a sphere given the radius
INPUT:
  r:sphere radius
OUTPUT:
  A=surface area *)

(* Compute the area of a sphere of radius r *)
A = 4.*Pi*r^2;

```