Lab 3

In this lab, we will practice the following topics on Mathematica:

- Compute sums
- Approximate definite integrals using Riemann sums
- Test and compare convergence rates of different Riemann sums
- Find improper integrals
- Find integrals that have undetermined parameters

The next lab will be built upon this lab, so please make sure that you go through all the instruction carefully and do all the assignments.

1 To turn in

Do Problems 1-26 in a single Mathematica Notebook file, or ipynb file if you use JupyterLab. Write *your name* and *lab number* at the beginning of your report. Clearly label each problem to separate them from other problems. Make sure to comment on each problem. If your code doesn't run correctly, explain what you are trying to do. **Failed code without any comment/explanation will receive 0 point.** Submit on Canvas both the *pdf file* and the *source file* (nb or ipynb).

Problems	Points
1, 2, 5, 17, 22-24	1
6, 7, 9, 11, 13, 25	2
3, 4, 8, 10, 12, 15, 16, 18-21	3
14	4
Readability of your report	3
Total: 26	Total: 62

2 Compute sums

1. To compute the sum $1 + \frac{1}{2} + \frac{1}{3} + ... + \frac{1}{10}$, you write it in *sigma notation* as $\sum_{k=1}^{10} \frac{1}{k}$. Then you can evaluate this sum as follows:

   ```
   Sum[1/k, {k,1,10}]
   ```

   With the command **Sum**, Mathematica will try to evaluate the sum exactly. If you want a result in form of decimal number, enclose the command inside the **N[...]** command. For example, to get an approximate value with 8 significant digits, try the following:

   ```
   N[Sum[1/k, {k,1,10}], 8]
   ```

2. To compute $2^2 - 3^2 + 4^2 - 5^2 + ... - 99^2 + 100^2$, we write this sum in sigma notation as $\sum_{k=2}^{100} (-1)^k k^2$. We can evaluate this formula with the command:

   ```
   Sum[(-1)^k*k^2, {k,2,100}]
   ```

3. Consider the sum $\frac{1}{3} + \frac{1}{5} + \frac{1}{7} + ... + \frac{1}{201}$. First, evaluate it exactly (your result will be a big fraction). Second, evaluate it in decimal form with 10 digits after the decimal point.

4. Do likewise for the sum $\frac{1}{3} - \frac{1}{5} + \frac{1}{7} - \frac{1}{9} + ... - \frac{1}{201}$.

3 Approximate definite integrals using Riemann sums

To evaluate the definite integral $\int_a^b f(x)dx$, it is a common practice to find an antiderivative of $f(x)$ by using substitution and/or integration by parts. However, not all functions have an antiderivative of elementary form. In such a case, we can still find approximate values of the definite integral using Riemann sums.

We do so by dividing the interval $[a, b]$ into n equal subintervals of length $\Delta x = \frac{b-a}{n}$. The grid-points are $x_0 = a$, $x_1 = a+\Delta x$, $x_2 = a+2\Delta x$,..., $x_n = a+n\Delta x = b$. In general, $x_k = a+k\Delta x$ for any k between 0 and n. As there are different ways to determine the height of the rectangular slats, there are different types of Riemann sums:

- Left endpoint Riemann sum:
$$L_n = \frac{b-a}{n}\sum_{k=1}^{n} f(x_{k-1})$$
- Right endpoint Riemann sum:
$$R_n = \frac{b-a}{n}\sum_{k=1}^{n} f(x_k)$$
- Midpoint Riemann sum:
$$M_n = \frac{b-a}{n}\sum_{k=1}^{n} f\left(\frac{x_{k-1}+x_k}{2}\right)$$
- Trapezoid Riemann sum:
$$T_n = \frac{b-a}{n}\sum_{k=1}^{n} \frac{f(x_{k-1})+f(x_k)}{2}$$

5. Knowing that the exact value of the integral
$$\int_1^2 x^2 dx$$
is $\frac{7}{3} = 2.333...$, it would be interesting to see how well these sums approximate this integral. We start by defining the function:

```
f[x_]:=x^2
a = 1
b = 2
```

Next, we will create a function called L which receives the values of a, b, n and returns the value the left endpoint Riemann sum L_n. In the formula of L_n mentioned above, keep in mind that $x_{k-1} = a+(k-1)\Delta x$ and $\Delta x = (b-a)/n$.

```
L[n_] :=  (b - a)/n * N[Sum[f[a + (k - 1)*(b - a)/n], {k, 1, n}], 12]
```

To find L_{10}, simply enter

```
L[10]
```

6. You can expect that as n increases, the Riemann sums L_n, R_n, M_n, T_n will better approximate the exact value of the integral
$$\int_1^2 x^2 dx$$

Let us make a table of 5 columns. The first column is the values of n. The second, third, fourth, fifth columns are the values of L_n, R_n, M_n, T_n, respectively. Different rows correspond to different values of n. Let n increase from 100 to 2100 with a jump of 200 from one row to the next.

```
Table[{n, L[n], R[n], M[n], T[n]}, {n, 100, 2100, 200}] // TableForm
```

Which of those four Riemann sums yields the best result? In other words, as n increases, which column has the fastest convergence to the exact value $\frac{7}{3} = 2.3333...$?

7. Put the heading on each column of the table in the previous exercise. *Hint: search Google for the phrase "put heading for table in mathematica".*

8. The error of approximation for the left endpoint Riemann sum is $\left|L_n - \frac{7}{3}\right|$. In Mathematica, you can type it as `Abs[L[n]-7/3]`. Modify the command in Exercise 6 to make a table of errors. To get an error less than 0.0005, how large must n be for each type of Riemann sums?

9. Do Exercises 6-8 for the integral
$$\int_0^{\pi} \cos(x^2)dx.$$
You may use different starting, ending, spacing values for n. Test if Mathematica can evaluate the integral exactly using **Integrate**. If not, you can use the approximate value from **N[Integrate[...], 12]** as the exact value.

The following error estimates are well-known in theory (see, for example, Section 7.7 of the textbook).

$$\begin{aligned}
E_L = \left|L_n - \int_a^b f(x)dx\right| &\leq \frac{(b-a)^2}{n} \max_{[a,b]} |f'| \\
E_R = \left|R_n - \int_a^b f(x)dx\right| &\leq \frac{(b-a)^2}{n} \max_{[a,b]} |f'| \\
E_M = \left|M_n - \int_a^b f(x)dx\right| &\leq \frac{(b-a)^3}{24n^2} \max_{[a,b]} |f''| \\
E_T = \left|T_n - \int_a^b f(x)dx\right| &\leq \frac{(b-a)^3}{12n^2} \max_{[a,b]} |f''|
\end{aligned}$$

An important consequence is that, as $n \to \infty$, E_L and E_R converge to 0 at the rate of $1/n$, whereas E_M and E_L converge to 0 at the rate of $1/n^2$, which is faster than $1/n$. The proofs of the above estimates are elementary but does require some clever tricks. You are not asked to prove them here. However, the exercises below will help you verify experimentally the rate of convergence just mentioned ($1/n$ and $1/n^2$). Roughly speaking, you can think of the above estimates as

$$E_L \approx \frac{C_1}{n}, \quad E_R \approx \frac{C_2}{n}, \quad E_M \approx \frac{C_3}{n^2}, \quad E_T \approx \frac{C_4}{n^2}$$

where C_1, C_2, C_3, C_4 are positive numbers depending on f but not on n. Apply the logarithm:

$$\ln E_L \approx \ln C_1 - \ln n, \quad \ln E_R \approx \ln C_2 - \ln n, \quad \ln E_M \approx \ln C_3 - 2\ln n, \quad \ln E_T \approx \ln C_4 - 2\ln n$$

Therefore, for large values of n, the points $(\ln n, \ln E_L)$ should approximately fit a straight line of slope -1. Likewise, the points $(\ln n, \ln E_M)$ should approximately fit a straight line of slope -2. This is what you expect to see in the following experiments.

10. Consider the integral $\int_1^2 x^2 dx$. Define the function f and the leftpoint Riemann sum L as in Exercise 5. Then define the error function E_L as

```
ev = Integrate[f[x], {x, a, b}];
EL[n_] := Abs[L[n] - ev];
```

Go ahead and define the error functions E_R, E_M, E_T in likewise manner.

11. You can plot the list of points $(\ln n, \ln E_L)$, for n from 10 to 20, as follows.

```
Ldata = Table[{Log[n], Log[EL[n]]}, {n, 10, 20}];
ListPlot[Ldata]
```

To find the line $y = ax + b$ that best fit this dataset, use the command

```
Fit[Ldata, {x, 1}, x]
```

What is the slope of this line? Increase the range of n (for example, n ranging from 100 to 150) and see what happens to the slope. Is what you observe consistent with the theoretical analysis mentioned earlier?

12. Do Exercise 11 for the right endpoint, midpoint, trapezoid Riemann sums. Name the corresponding datasets `Rdata, Mdata, Tdata`.

13. Draw all the datasets on the same plot using:

```
ListPlot[{Ldata, Rdata, Mdata, Tdata}, PlotLegends -> {"L", "R", "M", "T"}]
```

From the picture, explain why the lowest dataset corresponds to the least error (thus, the best method). *Hint: think of the relationship between* $E_{L,R,M,T}$ *and* $\ln E_{L,R,M,T}$.

14. Use experiment to find out which method, *midpoint sum* or *trapezoid sum*, is better for evaluating the integral $\int_0^\pi \cos(x^2)dx$.

Another method to approximate an integral is the Simpson's rule:

$$\int_a^b f(x)dx \approx S_n = \frac{b-a}{6n} \sum_{k=1}^{n} \left(f(x_{k-1}) + 4f\left(\frac{x_{k-1}+x_k}{2}\right) + f(x_k) \right)$$

15. Evaluate the integral $\int_0^\pi \cos(x^2)dx$ using the Simpson's rule with $n = 10$.

16. Follow the procedure in Exercise 11 to find out the convergence rate of the error of Simpson's rule for the integral $\int_0^\pi \cos(x^2)dx$. Is it $\frac{1}{n}$, $\frac{1}{n^2}$, or a higher power of $\frac{1}{n}$?

4 Improper integrals

17. In the command **Integrate**, you specify the integral bounds $\int_a^b$ by writing `{x,a,b}`. One or both of these bounds might be $\pm\infty$. Try the following:

```
Integrate[1/(x^2+1), {x,0,Infinity}]
N[Integrate[E^(-x^2), {x,-Infinity,0}], 10]
```

For Problems 18-21, do the following:

- Plot the integrand and explain why the integral is an improper integral.
- Add the option `Filling -> Axis` to your plot command to shade the region whose area is represented by the integral.
- Try to find the exact value of the integral using **Integrate**. If Mathematica fails to give you an answer, use **N[Integrate[...]]** to get an approximate value with 8 digits after the decimal point.

18. $\int_{-\infty}^{\infty} \frac{1}{x^2+1} dx$
19. $\int_{-\infty}^{1} e^x \sin x dx$
20. $\int_0^1 \ln(x) dx$
21. $\int_0^1 \sin\left(\frac{1}{x}\right) dx$

5 Integrals with unspecified parameters

Sometimes, the integrand may contain a parameter whose value is unspecified. Consider two following examples,

$$\int_0^{a/2} \frac{1}{x^2 - a^2} dx, \qquad \int_0^{\infty} \frac{1}{x^2 + a^2} dx$$

22. Find the first integral using **Integrate**.
23. Find the second integral using **Integrate**. You will see that, unlike the first integral, the result depends on whether $a > 0$, $a < 0$, or $a = 0$.

To specify an assumption on the parameter a, we add an option **Assumptions** inside the **Integrate** command. For example, to specify that $a > 0$, we write

```
Assumptions->{a>0}
```

To specify that a is a natural number, i.e. 1,2,3,4,..., we write

```
Assumptions->{a \[Element] PositiveIntegers}
```

To specify that $a > 0$ and n is a natural number, we write

```
Assumptions->{a>0, n \[Element] PositiveIntegers}
```

24. Try the command

```
Integrate[1/(x^2 + a^2), {x, 0, Infinity}, Assumptions -> a > 0]
```

25. In the above command, change the assumption to $a < 0$ and then $a = 0$ (double equal sign). What do you observe?
26. Find the integral

$$\int_0^{\infty} (a^2x^2 + b^2)^n \, dx$$

where $a < 0$, $b > 0$, and n is a negative integer.