1 Mathematics 406, Assignment 3’17 Due Oct 18

1. Integrals on infinite intervals: Consider evaluating the improper integrals:

\[ I_1 = \int_{-\infty}^{\infty} e^{-x^2} \cos x \, dx = \pi^{1/2}e^{-1/4} \]

\[ I_2 = \int_{-\infty}^{\infty} e^{-x^2} \cos^2 x \, dx = \pi^{1/2}(1 + e^{-1})/2 \]

(a) Since the integrands are symmetric convert the integration interval to \([0, \infty)\) and use your Romberg routine to estimate \(I_1\) and \(I_2\) as follows. Evaluate these integral directly by dividing the integral into two parts i.e. \([0, \infty) = [0, c] \cup [c, \infty)\). Can you control the error in the discarded part? What happens if you keep increasing \(c\)? Plot \(I_k(c)\).

Solution: Observe that

\[ \left| \int_{c}^{\infty} e^{-x^2} \cos x \, dx \right| < \int_{c}^{\infty} e^{-x^2} \, dx \]

and similarly with \(\cos^2 x\). Now to estimate \(\int_{c}^{\infty} e^{-x^2} \, dx\) consider the integral

\[ J(x) = e^{x^2} \int_{x}^{\infty} e^{-t^2} \, dt \]

then differentiating \(J(x)\) we obtain an ODE for \(J\) of the form

\[ J(x) = \frac{1}{2x} + \frac{1}{2x} J'(x) \]

This forms a recursion that generates the following asymptotic series for \(J(x)\) in the limit \(x \to \infty:\)

\[ J(x) = \frac{1}{2x} - \frac{1}{4x^3} + \cdots \]

which leads us to the estimate \(\int_{c}^{\infty} e^{-x^2} \, dx \sim \frac{e^{-c^2/2c}}{2c} < e^{-c^2}\). Thus in order that the discarded tail be less than \(10^{-8}\) we conclude that \(c \gtrsim (8 \ln 10)^{1/2} = 4.3\). In the graphs below the blue graph on the left side is the integral as a function of \(c\) while the red graphs represent \(\pi^{1/2}e^{-1/4} \pm \frac{e^{-c^2}}{2c}\) and \(\pi^{1/2}(1 + e^{-1})/2 \pm \frac{e^{-c^2}}{2c}\). The right graphs plot the error as a function of the truncation point \(c\). Since the Romberg integration routine uses a tolerance of \(10^{-8}\) the error no longer decreases beyond \(c \gtrsim 4.3\) as it is dominated by the Romberg error.
Integral $\int_0^c \exp(-x^2) \cos(x) \, dx$ using direct Romberg Integration

Integral $\int_0^c \exp(-x^2) \cos^2(x) \, dx$ using direct Romberg Integration
(b) Gauss-Hermite quadrature with integration points evaluates integrals of the form
\[ \int_{-\infty}^{\infty} e^{-x^2} f(x) dx \]

exactly if \( f(x) \) is a polynomial of degree \( 2m - 1 \). Use this fact to determine the integration points \( \xi_i \) and weights \( w_i \) in the formula
\[ \int_{-\infty}^{\infty} e^{-x^2} f(x) dx \approx w_1 f(\xi_1) + w_2 f(\xi_2) \text{ if } m = 2 \]
\[ \int_{-\infty}^{\infty} e^{-x^2} f(x) dx \approx w_1 f(\xi_1) + w_2 f(\xi_2) + w_3 f(\xi_3) \text{ if } m = 3 \]

To simplify your calculation, in the case \( m = 2 \) you may assume the symmetry conditions \( w_1 = w_2 \) and \( \xi_1 = -\xi_2 \), in the case \( m = 3 \), you may assume \( w_1 = w_3, \xi_2 = 0, \) and \( \xi_1 = -\xi_3 \).

Hint: It may also be helpful to know that \( \int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi} \), \( \int_{-\infty}^{\infty} e^{-x^2} x^2 dx = \frac{1}{2} \sqrt{\pi} \), and \( \int_{-\infty}^{\infty} e^{-x^2} x^4 dx = \frac{3}{4} \sqrt{\pi} \).

Use these Gauss-Hermite quadrature rules to evaluate \( I_k \) and complete the following table:

**Solution:**

<table>
<thead>
<tr>
<th>( m )</th>
<th>( f(x) = \cos x )</th>
<th>( f(x) = \cos^2 x )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>1.347498</td>
<td>1.024428</td>
</tr>
<tr>
<td>3</td>
<td>1.382033</td>
<td>1.249608</td>
</tr>
<tr>
<td><strong>Exact</strong></td>
<td><strong>1.380388</strong></td>
<td><strong>1.212252</strong></td>
</tr>
</tbody>
</table>
Q1(b) \( m = 2 \) since the Gauss-Hermite integration rule should integrate a polynomial of degree \( 2m - 1 = 3 \) exactly. Consider

\[ I = \int_{-\infty}^{\infty} e^{-x^2} \left[ a_0 + a_1 x^2 + a_2 x^4 + a_3 x^6 \right] dx = \frac{a_0 \sqrt{\pi}}{2} \]  

by the given integrals

\[ = w_1 \left[ f(-s_2) + f(s_2) \right] \text{ using the symmetry} \]

\[ = w_1 \left[ \left( a_0 - a_1 \frac{s_2^2}{2} + a_2 s_2^4 - a_3 \right) + \left( a_0 - a_1 \frac{s_2^2}{2} + a_2 s_2^4 + a_3 \right) \right] \]

\[ = 2w_1 a_0 + 2w_1 \frac{s_2^2}{2} a_2 \]

Equating coefficients:

\[
\begin{align*}
a_0 \quad &2w_1 = \sqrt{\pi} \quad w_1 = \sqrt{\pi}/2 \\
a_2 \quad &2w_1 \frac{s_2^2}{2} = \sqrt{\pi}/2 \Rightarrow (\sqrt{\pi}/2) \frac{s_2^2}{2} = \frac{\sqrt{\pi}}{2} \Rightarrow s_2^2 = \frac{1}{\sqrt{1/2}} = -s_1 \quad w_1 = \sqrt{\pi}/2
\end{align*}
\]

For \( m = 3 \): the G-H rule must integrate a polynomial of degree \( 2m - 1 = 5 \) exactly. So consider

\[ I = \int_{-\infty}^{\infty} e^{-x^2} \left[ a_0 + a_1 x^2 + a_2 x^4 + a_3 x^6 + a_4 x^8 \right] dx = \frac{a_0 \sqrt{\pi}}{2} + \frac{a_2 \sqrt{\pi}}{4} \]

\[ = w_1 \left[ f(-s_3) + f(s_3) \right] + w_2 f(s_3 = 0) \]

\[ = w_1 \left[ (a_0 - a_1 \frac{s_3^2}{4} + a_2 \frac{s_3^4}{16} - a_3 \frac{s_3^6}{64}) + (a_0 - a_1 \frac{s_3^2}{4} + a_2 \frac{s_3^4}{16} + a_3 \frac{s_3^6}{64}) \right] + w_2 a_0 \]

Equating coefficients:

\[
\begin{align*}
a_0 \quad &2w_1 + w_2 = \sqrt{\pi} \\
a_2 \quad &2w_1 \frac{s_3^2}{4} = \sqrt{\pi}/2 \Rightarrow (2w_1 \frac{s_3^2}{4}) \frac{s_3^2}{4} = \frac{\sqrt{\pi}}{2} \Rightarrow s_3^2 = \frac{1}{\sqrt{1/2}} = -s_1
\end{align*}
\]

Now \( 2w_1 \frac{s_3^2}{4} = 2w_1 (\frac{3}{2}) = \frac{\sqrt{\pi}}{4} \Rightarrow w_1 = \sqrt{\pi}/6 \)

\[ 2w_1 + w_2 = \sqrt{\pi} \Rightarrow w_2 = \sqrt{\pi} - \frac{\sqrt{\pi}}{3} = \frac{2\sqrt{\pi}}{3} \]
2. **Singular Integrals:** Evaluate the Fresnel integral \( I = \int_0^{\pi/2} x^{-\frac{1}{2}} \cos x \, dx = 1.95490284858266 \) directly using your Midpoint code. The convergence of the numerical approximation can be improved by subtracting out the singularity as follows: \( I = \int_0^{\pi/2} x^{-\frac{1}{2}} \, dx + \int_0^{\pi/2} x^{-\frac{1}{2}} (\cos x - 1) \, dx = (2\pi)^{\frac{1}{2}} + \int_0^{\pi/2} x^{-\frac{1}{2}} (\cos x - 1) \, dx. \) Since the last integrand is no longer singular it can be evaluated without difficulty using the routines developed above. Use the repeated Trapezoidal rule to evaluate \( I \) by subtracting one and three terms in the Taylor series expansion for \( \cos x \). Compare your results in the following table:

**SOLUTION:**

- 3 terms: \( I = \int_0^{\pi/2} x^{-\frac{1}{2}} - x^{\frac{3}{2}} + \frac{x^5}{6} \, dx + \int_0^{\pi/2} x^{-\frac{1}{2}} (\cos x - 1 + \frac{x^2}{2} - \frac{x^3}{6}) \, dx \)

<table>
<thead>
<tr>
<th>Integration Rule</th>
<th>( h = (\frac{\pi}{2})2^{-1} )</th>
<th>( h = (\frac{\pi}{2})2^{-6} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Direct Midpoint</td>
<td>1.765666396389619</td>
<td>1.860156095195565</td>
</tr>
<tr>
<td>Direct 3 pt Gauss</td>
<td>1.876839228294837</td>
<td>1.876839228294837</td>
</tr>
<tr>
<td>Subtract 1 term Midpoint</td>
<td>1.955096450291370</td>
<td>1.954915723360832</td>
</tr>
<tr>
<td>Subtract 1 term 3 pt Gauss</td>
<td>1.954903132541657</td>
<td>1.954902857457128</td>
</tr>
<tr>
<td>Subtract 1 term Trapezium</td>
<td>1.954504413769041</td>
<td>1.954876746967585</td>
</tr>
<tr>
<td>Subtract 3 terms Midpoint</td>
<td>1.955073566116061</td>
<td>1.954913499039223</td>
</tr>
<tr>
<td>Subtract 3 terms 3 pt Gauss</td>
<td>1.954902845667179</td>
<td>1.954902845667063</td>
</tr>
<tr>
<td>Subtract 3 terms Trapezium</td>
<td>1.954561691962987</td>
<td>1.954881549828570</td>
</tr>
</tbody>
</table>
3. **Duffy transformation**: Consider evaluating the following integral involving the Newtonian potential over a triangle

\[
I = \frac{1}{4\pi} \int_0^1 \int_0^x \sigma(x, y) \frac{dy}{(x^2 + y^2)^{1/2}} dx
\]  

(1)

which has a singularity at the vertex \( r = (x^2 + y^2)^{1/2} = 0 \).

(a) Show that the Duffy transformation from \((x, y) \rightarrow (x, u)\) given by \( u = y/x \) reduces the integration over the triangle to the following non-singular integral over the unit rectangle \((x, u) \in [0, 1] \times [0, 1]\).

\[
I = \frac{1}{4\pi} \int_0^1 \int_0^1 \sigma(x, xu) \frac{dxdu}{(1 + u^2)^{1/2}}
\]  

(2)

(b) For the special case \( \sigma(x, y) = 1 \) the integral has the exact value \( I = -\frac{1}{4\pi} \ln (\sqrt{2} - 1) = 0.881373587/4\pi \). Now implement a composite integration scheme with \( N \times N \) cells based on the \( 3 \times 3 \) product Gauss-Legendre quadrature rule to evaluate the integral in (2) and complete to following table:

<table>
<thead>
<tr>
<th>( N )</th>
<th>( 4\pi I )</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.8813312019380</td>
</tr>
<tr>
<td>2</td>
<td>0.8813734873142</td>
</tr>
<tr>
<td>3</td>
<td>0.8813735830245</td>
</tr>
<tr>
<td>4</td>
<td>0.8813735863282</td>
</tr>
<tr>
<td>5</td>
<td>0.8813735868391</td>
</tr>
<tr>
<td><em>Exact</em></td>
<td>0.8813735870195</td>
</tr>
</tbody>
</table>
4. Numerical evaluation of the Hankel transform: The zeroth order Hankel Transform

\[ \mathcal{H}_0(f; k) = \int_0^{\infty} f(r)J_0(kr)rdr \]

where \(J_0\) is the zeroth order Bessel function provides an efficient way to evaluate the 2D Fourier Transform of a circularly symmetric function. For the case \(f(r) = \frac{1}{(1+r^2)^{3/2}}\) the Hankel transform is

\[ \mathcal{H}_0\left(\frac{1}{(1+r^2)^{3/2}}; k\right) = e^{-k} \]

Use your Romberg routine to approximate \(\mathcal{H}_0\left(\frac{1}{(1+r^2)^{3/2}}; k\right)\) by the evaluating the above integral numerically for \(k = 3\) and \(k = 5\). Evaluate these integrals directly by dividing the integral into two parts i.e. \([0, \infty) = [0, c] \cup [c, \infty)\). Can you control the error in the discarded part? What happens if you keep increasing \(c\)? Plot \(I(c)\). How large must \(c\) be in order to achieve 4 digits of precision?

**Solution:** Replacing \(J_0(z)\) by its asymptotic behaviour \(J_0(z) \sim (\frac{\pi}{2z})^{1/2}\cos(z - \pi/4)\) as \(z \to \infty\), we obtain the estimate

\[ \int_c^{\infty} \frac{J_0(kr)r}{(1+r^2)^{3/2}}dr \lesssim \int_c^{\infty} r^{-5/2}dr = \frac{2}{3} c^{-3/2} < Tol \tag{3} \]

If we require a truncation error that is less than \(10^{-4}\) for example we would need \(c \geq (\frac{2}{7}10^{-4})^{-2/3} \approx 354\) to guarantee this accuracy using (3). From the graphs of \(I(c)\) below we observe multiple oscillations even for relatively large values of \(c\), which is more extreme for \(k = 5\) than for \(k = 3\). From the relative error plots \(I(c) - e^{-k}/e^{-k}\) we observe that for \(k = 3\) we can expect four digits of precision for \(c > 60\), while for \(k = 5\) we can expect four digits of precision for \(c > 100\). These bounds are confirmed by the results in the table below.

<table>
<thead>
<tr>
<th>(k)</th>
<th>(3)</th>
<th>(5)</th>
</tr>
</thead>
<tbody>
<tr>
<td>(c = 10)</td>
<td>0.049428442</td>
<td>0.006539984</td>
</tr>
<tr>
<td>(c = 20)</td>
<td>0.049829432</td>
<td>0.006699255</td>
</tr>
<tr>
<td>(c = 50)</td>
<td>0.049778393</td>
<td>0.006734513</td>
</tr>
<tr>
<td>(c = 100)</td>
<td>0.049786017</td>
<td>0.006738160</td>
</tr>
<tr>
<td>Exact</td>
<td>0.049787068</td>
<td>0.006737946</td>
</tr>
</tbody>
</table>

The value of \(c\) required by the bound (3) is over-conservative as it ignores the more rapid convergence of the actual integral due to oscillations.