Project 2

Math 400, Spring 2025
Due Wed 05/07
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1. This is a problem on Gaussian quadrature and related things.

   a. Explain the principle of the Gaussian quadrature.

   Sol:

   The Gaussian quadrature principle selects n nodes x_i and weights c_i such that the formula $\int_{-1}^{1} f(x)\,dx \approx \sum_{i=0}^{n-1} c_i f(x_i)$ is exact for polynomials of the highest possible degree. For n nodes, it achieves exactness for polynomials up to degree $2n-1$. The nodes are roots of orthogonal polynomials such as the Legendre polynomials, and the weights ensure exact integration for lower-degree polynomials.

   b. Show that the Gaussian quadrature $\int_{-1}^{1} f(x)dx = c_0 f(x_0) + c_1 f(x_1)$ can be exact for all polynomials of degree 3 with 2 points $x_0 = -\frac{1}{\sqrt{3}}$ and $x_1 = \frac{1}{\sqrt{3}}$. Find c_0 and c_1 as well.

   Sol:

   - For $f(x) = 1$:

   $$\int_{-1}^{1} 1\,dx = 2 \implies c_0 + c_1 = 2$$

   - For $f(x) = x$:

   $$\int_{-1}^{1} x\,dx = 0 \implies c_0\left(-\frac{1}{\sqrt{3}}\right) + c_1\left(\frac{1}{\sqrt{3}}\right) = 0 \implies c_0 = c_1$$

   Solving $c_0 + c_1 = 2$ and $c_0 = c_1$, we get $c_0 = c_1 = 1$.

   - Verification for $f(x) = x^2$:

   $$\int_{-1}^{1} x^2\,dx = \frac{2}{3} \quad \text{and} \quad 1\cdot\left(\frac{1}{\sqrt{3}}\right)^2 + 1\cdot\left(-\frac{1}{\sqrt{3}}\right)^2 = \frac{2}{3}$$

   - Verification for $f(x) = x^3$:

   $$\int_{-1}^{1} x^3\,dx = 0 \quad \text{and} \quad 1\cdot\left(\frac{1}{\sqrt{3}}\right)^3 + 1\cdot\left(-\frac{1}{\sqrt{3}}\right)^3 = 0$$

   From this, we get:

   $$\boxed{c_0 = 1}, \quad \boxed{c_1 = 1}$$

   c. Determine the values of c_i and $x_i, i = 0, 1$ so that the quadrature formula $\int_{-1}^{1} x^2 f(x)dx = c_0 f(x_0) + c_1 f(x_1)$ will be exact for all polynomials of degree 3.

- For $f(x) = 1$:

$$\int_{-1}^{1} x^2\,dx = \frac{2}{3} = c_0 + c_1 \implies c_0 + c_1 = \frac{2}{3}$$

- For $f(x) = x$:

$$\int_{-1}^{1} x^3\,dx = 0 = c_0 x_0 + c_1 x_1$$

- For $f(x) = x^2$:

$$\int_{-1}^{1} x^4\,dx = \frac{2}{5} = c_0 x_0^2 + c_1 x_1^2$$

- For $f(x) = x^3$:

$$\int_{-1}^{1} x^5\,dx = 0 = c_0 x_0^3 + c_1 x_1^3$$

Assume symmetry $x_1 = -x_0$. Then $c_0 = c_1$, and $c_0 = c_1 = \frac{1}{3}$. Substituting into $c_0 x_0^2 + c_1 x_1^2 = \frac{2}{5}$:

$$\frac{2}{3} x_0^2 = \frac{2}{5} \implies x_0 = \sqrt{\frac{3}{5}}$$

$$\boxed{c_0 = \frac{1}{3}}, \quad \boxed{c_1 = \frac{1}{3}}, \quad \boxed{x_0 = \sqrt{\frac{3}{5}}}, \quad \boxed{x_1 = -\sqrt{\frac{3}{5}}}$$

2. Mass spectrometry analysis gives a series of peak height readings for various ion masses. For each peak, the height h_i is contributed to by various constituents (measured by the index j). The j^{th} component with per unit concentration p_j makes the contribution c_{ij} to the i^{th} peak, so that the relation $h_i = \sum_{j=1}^{n} c_{ij} p_j$ holds. n is the number of components present. Carnahan (1964) gives the c_{ij} values shown in the table below:

Peak number	Unknown	CH_4	C_2H_4	C_2H_6	C_3H_6	C_3H_8
1		0.165	0.202	0.317	0.234	0.182
2		27.7	0.862	0.062	0.073	0.131
3			22.35	13.05	4.42	6.001
4				11.28	0	1.11
5					9.85	1.684

If a sample had measured peak heights $h_i = 5.20, h_2 = 61.7, h_3 = 149.2, h_4 = 79.4$, and $h_5 = 89.3$. Calculate the values of p_j for each component. The total of all the p_j values was 51.53. Use Jacobi's and Gauss-Seidel iteration approaches, till adjacent iterations is within 10^{-6}.

Requirements: Rearrange the measurements to take advantages of the principle and strength of each iteration method.

Sol:

Unknown :	30.0696
CH_4 :	2.1701
C_2H_4 :	0.0000
C_2H_6 :	6.6100
C_3H_6 :	8.3206
C_3H_8 :	4.3597
Total :	51.53