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MA 322: Scientific Computing Lab

Lab 05

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Using the Gaussian Quadrature Rule...

The recurrence relation for $\phi_n(x)$ is given as:

$\phi_{n+1}(x) = (x - \alpha_n)\phi_n(x) - \beta_n\phi_{n-1}(x)$, and with the initial conditions as, $\phi_0(x) = 1,\ \phi_{-1}(x) = 0$. Also,

$\alpha_n = \frac{<x\phi_n,\, \phi_n>}{<\phi_n,\, \phi_n>}$ *and* $\beta_n = \frac{<\phi_n,\, \phi_n>}{<\phi_{n-1},\, \phi_{n-1}>}$

From this, we can define the Jacobi matrix as -

Define the Jacobi matrix

$$A = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & \\ & \sqrt{\beta_2} & \ddots & \ddots & \\ & & \ddots & \ddots & \sqrt{\beta_{n-1}} \\ & & & \sqrt{\beta_{n-1}} & \alpha_n \end{bmatrix}.$$

Then $\phi_{n+1}(x_j) = 0 \iff \det(A - x_j I) = 0$. Let $\mathbf{v_0}, \ldots, \mathbf{v_n}$ be orthonormal eigenvectors of A. Then $w_j = \langle 1,\, 1\rangle(\mathbf{e}_0^T\mathbf{v}_j)^2,\ j = 0 : n,$ are the required weights for the Gaussian quadrature rule

$$\int_a^b f(x)\mu(x)dx \approx w_0 f(x_0) + \cdots + w_n f(x_n).$$

Gaussian Quadrature by Dr B. Deka, IIT Guwahati

Using the procedure as above we write the code in python to compute weights, and then finally calculate the Gaussian quadrature as

$$G_n(f) = w_0 f(x_0) + \ldots + w_n f(x_n)$$

Question 1.

In this question, we use the Gaussian Quadrature rule with n=2 and approximate the given integrals.
In each case, we find the actual integral value and also compute the error in the approximation.

```
(a) Using Gaussian Quadrature with n = 2
Approximate value of integral is 0.19225937725687903
Exact value of the integral is 0.192259357732796
Error in estimation is 1.95240829614640E-8

(b) Using Gaussian Quadrature with n = 2
Approximate value of integral is -0.17682001788622057
Exact value of the integral is -0.176820020121789
Error in estimation is 2.23556864686891E-9

(c) Using Gaussian Quadrature with n = 2
Approximate value of integral is 0.0887538536178567
Exact value of the integral is 0.0887552844352566
Error in estimation is 0.0000014308173989448
```

Question 2.

We don't need a code for this question.
The solution has been attached in the form of 2 images on the following pages:

Question 02.

Given nodes $x_1, x_2, x_3, \ldots x_n \in [a, b]$, and, weights $w_1, w_2, w_3, \ldots w_n \in \mathbb{R}$ of a quadrature formula

Since $w_j < 0$ for some $j \in 1, 2, \ldots n$, assume $k_1, k_2, \ldots k_m \in 1, 2, \ldots n$, such that

$$w_{k_i} \geq 0 \ \forall \ 1 \leq i \leq m.$$

Also, let the set $\boxed{K = \{k_1, k_2, \ldots k_m\}}$ —— (A)

Define $f(x) = \prod_{i \in K} (x - x_i)^2$

$$\Rightarrow f(x) \geq 0 \quad \forall x \in [a, b]$$

Clearly $f(x)$ is a polynomial function and is thus continuous. Also, $f(x) > 0 \ \forall \ i \notin K$, thus

$\int_a^b f(x)\,dx > 0$, i.e. the integration would be positive.

Now, $\sum_{i=1}^{n} w_i f(x_i)$

$$= \sum_{i \in K} w_i f(x_i) + \sum_{i \notin K} w_i f(x_i)$$

But from (A), $f(x_i) = 0 \ \forall \ i \in K$.

$$\Rightarrow \sum_{i=1}^{n} w_i f(x_i) = \sum_{i \notin K} w_i f(x_i)$$

Now, when $i \notin k$,

a) $f(x_i) > 0 \quad \forall\, i \notin k$

b) $w_i < 0 \quad \forall\, i \notin k$.

$\Rightarrow \quad w_i f(x_i) < 0 \quad \forall\, i \notin k$

$\Rightarrow \quad \sum_{i \notin k} w_i f(x_i) < 0 \quad \forall\, i \notin k$.

and we know $\sum_{i \in k} w_i f(x_i) = 0 \quad \forall\, i \in k$.

$$\Rightarrow \boxed{\sum_{i=1}^{n} w_i f(x_i) < 0.}$$

So, the function $\boxed{f(x) = \prod_{i \in K} (x - x_i)^2}$ is a continuous function,

such that,

$f(x) \geq 0 \quad \forall\, x \in [a, b]$.

i.e. $\boxed{\int_a^b f(x)\, dx > 0, \text{ but } \sum_{i=1}^{n} w_i f(x_i) < 0}$

Question 3.

We use the 2 point Gaussian Quadrature rule and then Trapezoidal and Simpson's rules, we get :

```
Using 2 point Gaussian Quadrature rule approx. value of
integral is 1.0909090909090908
Using Trapezoidal rule approximate value of the integral is
1.3333333333333333
Using Simpson rule approximate value of the integral is
1.1111111111111111
Actual value of integral is 1.09861228866811
```

Also, the errors in estimation can be found out using `abs(actual value - estimated value)` as:

```
Error in estimation for Gaussian Quadrature rule =
0.007703197759018950
Error in estimation for Trapezoidal rule =
0.234721044665223
Error in estimation for Simpson rule = 0.0124988224430014
```

We can clearly observe that the 2-point Gaussian Quadrature rule gives better approximations as compared to Trapezoidal and Simpson's rules.

Question 4.

In this question, we make use of 3 points Gaussian Quadrature and Simpson's composite rule with h = 0.125.

The composite Simpson rule is given as:

$$S(f) = \frac{h}{3}[f(x_0) + 2\sum_{j=2}^{n/2} f(x_{2j-2}) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + f(x_n)]$$

We obtain:

```
Using 3 point Gaussian Quadrature rule approx. value of
integral is 0.693121693121693
Using Simpsons 1/3 rule with h = 0.125 approximate value of
the integral is 0.6931545306545307
Actual value of the integral is 0.693147180559945
```

Also, the errors in estimation can be found out using `abs(actual value - estimated value)` as:

```
Error in estimation for Gaussain Quadrature rule =
0.000025487438252585
Error in estimation for Simpsons rule =
0.00000735009458541214
```

We observe that Simpson's rule gives a better approximation (lower error) in this case as compared to the Gaussian Quadrature formula.

Question 5.

We don't need a code for this question.

```
Answer: The second formula is better.
The following 2 points summarise the reason.
  ● The values of the function at a and b are high, thus the
    first equation will lead to a significant deviation from
    the exact result. However, this won't happen if the second
    equation is used.

  ● Since n = 2, the value of h will be high. This implies the
    error term due to both approximations will be significant.
    Since the second equation follows the Open Newton Cotes
    formula, while the first one follows a Closed Newton Cotes
    formula, in such a scenario as above, the second equation
    will lead to a lower error!
```

Question 6.

In this question, we will make use of the n-points Gaussian Quadrature rule for n=1,2,3,4,5 to approximate the integral to 2 decimal places. The same has been done in the table below.

```
N       Evaluated value using N+1 point Gaussian Quadrature
```

```
1                                                -0.76
2                                                -0.84
3                                                -0.87
4                                                -0.88
5                                                -0.89
```

The actual value of the integral is ~ **–0.91596559**. We see with an increase in n the approximation by the Gaussian Quadrature becomes more accurate.