Fall, 2024 **06-606**

Nonlinear Optimization in Process Systems Engineering

Due: 11/15/24

1. For $\alpha = 4$ and for $\alpha = 100$ solve the problem presented in class:

$$u'' - \alpha u = 4t^2 - 2$$
$$u'(0) = 0,\ u(1) = 0$$

a) analytically
b) using finite differences with h = 0.1
c) using 2 pt. Collocation
d) single shooting

Legendre roots for collocation are given in the handout for $-1 \le z \le 1$ (and appended below). For this problem, we need to scale these roots between zero and one, so the collocation points can be found from: $t_i = 1/2(1 + z_i)$.

2. Apply 5 point global collocation to the problem below and solve:

$$1/r^2\ \partial/\partial r(r^2\ \partial c/\partial r) = (c(r))^2$$

$$\partial c/\partial r = 0 \text{ at } r = 0$$
$$\partial c/\partial r = 100(c(1) - 1) \text{ at } r = 1$$

3. Solve problem 3 using finite differences with h = 0.1, h = 0.01 and h = 0.001.

4. Solve problem 2 using GAMS or Python with a small number of collocation points (say, 3) and a set of number of finite elements (5 to 100) and assess the accuracy of these solutions. A Dynamic GAMS Example template can be found on http://numero.cheme.cmu.edu/course/06606.html.

Legendre-Gauss quadrature is a numerical integration method also called "the" Gaussian quadrature or Legendre quadrature. A Gaussian quadrature over the interval $[-1, 1]$ with weighting function $W(x) = 1$. The abscissas for quadrature order n are given by the roots of the Legendre polynomials $P_n(x)$, which occur symmetrically about 0. The weights are

$$w_i = -\frac{A_{n+1}\,\gamma_n}{A_n\,P_n'(x_i)\,P_{n+1}(x_i)} \tag{1}$$

$$= \frac{A_n}{A_{n-1}}\,\frac{\gamma_{n-1}}{P_{n-1}(x_i)\,P_n'(x_i)}, \tag{2}$$

where A_n is the coefficient of x^n in $P_n(x)$. For Legendre polynomials,

$$A_n = \frac{(2\,n)!}{2^n\,(n!)^2} \tag{3}$$

(Hildebrand 1956, p. 323), so

$$\frac{A_{n+1}}{A_n} = \frac{[2\,(n+1)]!}{2^{n+1}\,[(n+1)!]^2}\,\frac{2^n\,(n!)^2}{(2\,n)!} \tag{4}$$

$$= \frac{2\,n+1}{n+1}. \tag{5}$$

Additionally,

$$\gamma_n = \int_{-1}^{1} [P_n(x)]^2\,d\,x \tag{6}$$

$$= \frac{2}{2\,n+1} \tag{7}$$

(Hildebrand 1956, p. 324), so

$$w_i = -\frac{2}{(n+1)\,P_{n+1}(x_i)\,P_n'(x_i)} \tag{8}$$

$$= \frac{2}{n\,P_{n-1}(x_i)\,P_n'(x_i)}. \tag{9}$$

Using the recurrence relation

$$\left(1-x^2\right)P_n'(x) = -n\,x\,P_n(x) + n\,P_{n-1}(x) \tag{10}$$

$$= (n+1)\,x\,P_n(x) - (n+1)\,P_{n+1}(x) \tag{11}$$

$$\tag{12}$$

(correcting Hildebrand 1956, p. 324) gives

$$w_i = \frac{2}{\left(1-x_i^2\right)\left[P_n'(x_i)\right]^2} \tag{13}$$

$$= \frac{2\left(1-x_i^2\right)}{(n+1)^2\,[P_{n+1}(x_i)]^2} \tag{14}$$

(Hildebrand 1956, p. 324).

The weights w_i satisfy

$$\sum_{i=1}^{n} w_i = 2, \tag{15}$$

which follows from the identity

$$\sum_{\nu=1}^{n} \frac{1-x_\nu^2}{(n+1)^2\,[P_{n+1}(x_\nu)]^2} = 1. \tag{16}$$

The error term is

$$E = \frac{2^{2n+1}(n!)^4}{(2n+1)[(2n)!]^3} f^{(2n)}(\xi). \quad (17)$$

Beyer (1987) gives a table of abscissas and weights up to $n = 16$, and Chandrasekhar (1960) up to $n = 8$ for n even.

n	x_i	w_i
2	± 0.57735	1.000000
3	0	0.888889
	± 0.774597	0.555556
4	± 0.339981	0.652145
	± 0.861136	0.347855
5	0	0.568889
	± 0.538469	0.478629
	± 0.90618	0.236927

The exact abscissas are given in the table below.

n	x_i	w_i
2	$\pm \frac{1}{3}\sqrt{3}$	1
3	0	$\frac{8}{9}$
	$\pm \frac{1}{5}\sqrt{15}$	$\frac{5}{9}$
4	$\pm \frac{1}{35}\sqrt{525 - 70\sqrt{30}}$	$\frac{1}{36}\left(18 + \sqrt{30}\right)$
	$\pm \frac{1}{35}\sqrt{525 + 70\sqrt{30}}$	$\frac{1}{36}\left(18 - \sqrt{30}\right)$
5	0	$\frac{128}{225}$
	$\pm \frac{1}{21}\sqrt{245 - 14\sqrt{70}}$	$\frac{1}{900}\left(322 + 13\sqrt{70}\right)$
	$\pm \frac{1}{21}\sqrt{245 + 14\sqrt{70}}$	$\frac{1}{900}\left(322 - 13\sqrt{70}\right)$

The abscissas for order n quadrature are roots of the Legendre polynomial $P_n(x)$, meaning they are algebraic numbers of degrees 1, 2, 2, 4, 4, 6, 6, 8, 8, 10, 10, 12, ..., which is equal to $2\lfloor n/2 \rfloor$ for $n > 1$ (Sloane's A052928).

Similarly, the weights for order n quadrature can be expressed as the roots of polynomials of degree 1, 1, 1, 2, 2, 3, 3, 4, 4, 5, 5, ..., which is equal to $\lfloor n/2 \rfloor$ for $n > 1$ (Sloane's A008619). The triangle of polynomials whose roots determine the weights is

$$x - 2 \quad (18)$$

$$x - 1 \quad (19)$$

$$9x - 5 \quad (20)$$

$$216x^2 - 216x + 49 \quad (21)$$

$$45000x^2 - 32200x + 5103 \quad (22)$$

$$2025000x^3 - 2025000x^2 + 629325x - 58564 \quad (23)$$

$$142943535000x^3 - 113071253400x^2 + 27510743799x - 1976763932 \quad (24)$$

$$1707698764800000x^4 - 1707698764800000x^3 + 606530263046400x^2 - 88878097916608x + 4373849390625 \quad (25)$$

(Sloane's A112734).

REFERENCES:

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Chandrasekhar, S. *Radiative Transfer.* New York: Dover, pp. 56-62, 1960.

Hildebrand, F. B. *Introduction to Numerical Analysis.* New York: McGraw-Hill, pp. 323-325, 1956.

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