Orthogonal Collocation Parameters

ref: Finlayson, B. A., "Nonlinear Analysis in Chemical Engineering", p192ff, McGraw-Hill, 1980

Finlayson Section 4-7

Problem specification

$N := 6$

The number of interior collocation points. This number can not be changed without manual changes to the g(x,c) function and the solve block.

$a := 3$

geometry parameter

- 1 = planar
- 2 = cylindrical
- 3 = spherical

The "a" parameter setting is enabled here to create a fully computed file for the PDF version. Normally this parameter is set in the calling program. That allows this file to be used for spherical catalyst pellets in Example 4 and cylindrical tubes in Examples 7 and 10.

$W(x) := 1 - x^2$

weighting function for orthogonal polynomials

Polynomials

$$g(x,c) := \begin{bmatrix} \sum_{j=0}^{0} \left(c_{0,j} \cdot x^{2 \cdot j}\right) \\ \sum_{j=0}^{1} \left(c_{1,j} \cdot x^{2 \cdot j}\right) \\ \sum_{j=0}^{2} \left(c_{2,j} \cdot x^{2 \cdot j}\right) \\ \sum_{j=0}^{3} \left(c_{3,j} \cdot x^{2 \cdot j}\right) \\ \sum_{j=0}^{4} \left(c_{4,j} \cdot x^{2 \cdot j}\right) \\ \sum_{j=0}^{5} \left(c_{5,j} \cdot x^{2 \cdot j}\right) \\ \sum_{j=0}^{6} \left(c_{6,j} \cdot x^{2 \cdot j}\right) \end{bmatrix} \rightarrow \begin{pmatrix} c_{0,0} \\ c_{1,1} \cdot x^{2} + c_{1,0} \\ c_{2,2} \cdot x^{4} + c_{2,1} \cdot x^{2} + c_{2,0} \\ c_{3,3} \cdot x^{6} + c_{3,2} \cdot x^{4} + c_{3,1} \cdot x^{2} + c_{3,0} \\ c_{4,4} \cdot x^{8} + c_{4,3} \cdot x^{6} + c_{4,2} \cdot x^{4} + c_{4,1} \cdot x^{2} + c_{4,0} \\ c_{5,5} \cdot x^{10} + c_{5,4} \cdot x^{8} + c_{5,3} \cdot x^{6} + c_{5,2} \cdot x^{4} + c_{5,1} \cdot x^{2} + c_{5,0} \\ c_{6,6} \cdot x^{12} + c_{6,5} \cdot x^{10} + c_{6,4} \cdot x^{8} + c_{6,3} \cdot x^{6} + c_{6,2} \cdot x^{4} + c_{6,1} \cdot x^{2} + c_{6,0} \end{pmatrix}$$

Determination of c matrix

Initial guesses

$i := 0..N \qquad j := 0..N$

$c_{i,j} := 0$

$c_{i,0} := 1$ The first column is 1 by definition.

$$c = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix}$$

Solve block

orthogonal constraints for the polynomial functions,g

Given

$$\int_0^1 W(x)\cdot g(x,c)_0\cdot g(x,c)_1\cdot x^{a-1}\,dx = 0$$

$$\int_0^1 W(x)\cdot g(x,c)_0\cdot g(x,c)_2\cdot x^{a-1}\,dx = 0 \qquad \int_0^1 W(x)\cdot g(x,c)_1\cdot g(x,c)_2\cdot x^{a-1}\,dx = 0$$

$$\int_0^1 W(x)\cdot g(x,c)_0\cdot g(x,c)_3\cdot x^{a-1}\,dx = 0 \qquad \int_0^1 W(x)\cdot g(x,c)_1\cdot g(x,c)_3\cdot x^{a-1}\,dx = 0$$

$$\int_0^1 W(x)\cdot g(x,c)_0\cdot g(x,c)_4\cdot x^{a-1}\,dx = 0 \qquad \int_0^1 W(x)\cdot g(x,c)_1\cdot g(x,c)_4\cdot x^{a-1}\,dx = 0$$

$$\int_0^1 W(x)\cdot g(x,c)_0\cdot g(x,c)_5\cdot x^{a-1}\,dx = 0 \qquad \int_0^1 W(x)\cdot g(x,c)_1\cdot g(x,c)_5\cdot x^{a-1}\,dx = 0$$

$$\int_0^1 W(x)\cdot g(x,c)_0\cdot g(x,c)_6\cdot x^{a-1}\,dx = 0 \qquad \int_0^1 W(x)\cdot g(x,c)_1\cdot g(x,c)_6\cdot x^{a-1}\,dx = 0$$

$$\int_0^1 W(x)\cdot g(x,c)_2\cdot g(x,c)_3\cdot x^{a-1}\,dx = 0$$

$$\int_0^1 W(x)\cdot g(x,c)_2\cdot g(x,c)_4\cdot x^{a-1}\,dx = 0 \qquad \int_0^1 W(x)\cdot g(x,c)_3\cdot g(x,c)_4\cdot x^{a-1}\,dx = 0$$

$$\int_0^1 W(x)\cdot g(x,c)_2\cdot g(x,c)_5\cdot x^{a-1}\,dx = 0 \qquad \int_0^1 W(x)\cdot g(x,c)_3\cdot g(x,c)_5\cdot x^{a-1}\,dx = 0$$

$$\int_0^1 W(x)\cdot g(x,c)_4\cdot g(x,c)_5\cdot x^{a-1}\,dx = 0$$

$$\int_0^1 W(x)\cdot g(x,c)_2\cdot g(x,c)_6\cdot x^{a-1}\,dx = 0 \qquad \int_0^1 W(x)\cdot g(x,c)_3\cdot g(x,c)_6\cdot x^{a-1}\,dx = 0 \qquad \int_0^1 W(x)\cdot g(x,c)_4\cdot g(x,c)_6\cdot x^{a-1}\,dx = 0 \qquad \int_0^1 W(x)\cdot g(x,c)_5\cdot g(x,c)_6\cdot x^{a-1}\,dx = 0$$

The following are given values as constraints.

$c_{0,0} = 1$ $c_{0,1} = 0$ $c_{0,2} = 0$ $c_{0,3} = 0$ $c_{0,4} = 0$ $c_{0,5} = 0$ $c_{0,6} = 0$

$c_{1,0} = 1$ $c_{1,2} = 0$ $c_{1,3} = 0$ $c_{1,4} = 0$ $c_{1,5} = 0$ $c_{1,6} = 0$

$c_{2,0} = 1$ $c_{2,3} = 0$ $c_{2,4} = 0$ $c_{2,5} = 0$ $c_{2,6} = 0$

$c_{3,0} = 1$ $c_{3,4} = 0$ $c_{3,5} = 0$ $c_{3,6} = 0$

$c_{4,0} = 1$ $c_{4,5} = 0$ $c_{4,6} = 0$

$c_{5,0} = 1$ $c_{5,6} = 0$

$c_{6,0} = 1$

$$c := \text{Find}(c) = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & -2.333 & 0 & 0 & 0 & 0 & 0 \\ 1 & -6 & 6.6 & 0 & 0 & 0 & 0 \\ 1 & -11 & 28.6 & -20.429 & 0 & 0 & 0 \\ 1 & -17.333 & 78 & -126.286 & 66.651 & 0 & 0 \\ 1 & -25 & 170 & -461.429 & 538.333 & -225.121 & 0 \\ 1 & -34 & 323 & -1.292 \times 10^{3} & 2.476 \times 10^{3} & -2.251 \times 10^{3} & 779.266 \end{pmatrix}$$

Find locations of x roots

Use the coefficients from the bottom row of c matrix (highest degree polynomial) to find the roots.

$$v1 := \left(c^{T}\right)^{\langle N \rangle} \qquad v1 = \begin{pmatrix} 1 \\ -34 \\ 323 \\ -1.292 \times 10^{3} \\ 2.476 \times 10^{3} \\ -2.251 \times 10^{3} \\ 779.266 \end{pmatrix}$$

$$h(x) := \begin{pmatrix} 1 \\ x^2 \\ x^4 \\ x^6 \\ x^8 \\ x^{10} \\ x^{12} \end{pmatrix}$$

define the polynomial functions in x

$$f(x) := v1^T \cdot h(x)$$

create the polynomial

$$v2 := f(x)\ \text{coeffs} \rightarrow \begin{pmatrix} 1 \\ 0 \\ -33.999999999999126 \\ 0 \\ 322.99999999998818 \\ 0 \\ -1291.9999999999486 \\ 0 \\ 2476.3333333332384 \\ 0 \\ -2251.2121212120437 \\ 0 \\ 779.26573426571144 \end{pmatrix}$$

Determine the coefficients in an expanded polynomial that would include the odd powers of x. Note the zeros were obtained for the odd powers.

$x := \text{polyroots}(v2)$ find the roots of the expanded polynomial

$x^T =$

	0	1	2	3	4	5	6	7	8	9	10	11
0	-0.965	-0.885	-0.764	-0.606	-0.421	-0.215	0.215	0.421	0.606	0.764	0.885	0.965

$x := \text{submatrix}(x, N, 2 \cdot N - 1, 0, 0)$ select the positive roots

$$x = \begin{pmatrix} 0.215 \\ 0.421 \\ 0.606 \\ 0.764 \\ 0.885 \\ 0.965 \end{pmatrix}$$

$x := \text{stack}(x, 1)$ add the location at x=1

Coefficient matrices for radial dispersion or diffusion problem

Finlayson formulas assume ORIGIN=1 for array indexes. The formulas below assume ORIGIN=0.

$i := 0 .. N$ this is the index for the polynomial terms

$j := 0 .. N$ this is the index for the collocation points

In the relationships below, the collocation form on the right side of the equal sign is substituted for the form on the left. E.g.. either $C \cdot d$ or $A \cdot Y$ may be substituted for $\frac{d}{dx} Y$ in a model.

$C_{j,i} := (2 \cdot i) \cdot \left(x_j\right)^{2 \cdot i - 1}$ coefficients in first derivative in x (radial direction)

used for: $\frac{d}{dx} Y = C \cdot d$

where d is vector of coefficients in polynomial

$Q_{j,i} := \left(x_j\right)^{2\cdot i}$ used for: $Y = Q\cdot d$

$A := C\cdot Q^{-1}$ used for: $\frac{d}{dx}Y = A\cdot Y$

$D_{j,i} := 2\cdot i\cdot(2\cdot i - 1 + a - 1)\cdot\left(x_j\right)^{2\cdot i-2}$ used for : $\frac{1}{x^{a-1}}\cdot\left[\frac{d}{dx}\left[x^{a-1}\cdot\left(\frac{d}{dx}Y\right)\right]\right] = D\cdot d$

$B := D\cdot Q^{-1}$ used for: $\frac{1}{x^{a-1}}\cdot\left[\frac{d}{dx}\left[x^{a-1}\cdot\left(\frac{d}{dx}Y\right)\right]\right] = B\cdot Y$

$f_i := \frac{1}{2\cdot i + a}$ see eq. 4-207 , Finlayson, p 95

$Wq := \left(f^T Q^{-1}\right)^T$ used for: $\int_0^1 f\left(x^2\right)\cdot x^{a-1}\,dx = \sum_{j=0}^{N}\left[Wq_j\cdot f\left[\left(x_j\right)^2\right]\right]$ weighting vector for quadrature integration formulas

Thus, if T_j is known (temperatures at the collocation point,, then the average temperature over the x dimension is given by:

$$T_{ave} = \frac{\int_0^1 T(x)\cdot x^{a-1}\,dx}{\int_0^1 x^{a-1}\,dx} = \frac{\int_0^1 T(x)\cdot x^{a-1}\,dx}{\frac{1}{a}}$$ by definition

The equivalent using the quadrature vector $T_{ave} = a\cdot\sum_{j=0}^{N}\left(Wq_j\cdot T_j\right)$

or in matrix notation: $T_{ave} = a\cdot Wq^T\cdot T$

Some examples of the computed values of the collocation matrices.

$$Wq = \begin{pmatrix} 9.831 \times 10^{-3} \\ 0.035 \\ 0.064 \\ 0.082 \\ 0.08 \\ 0.054 \\ 9.524 \times 10^{-3} \end{pmatrix}$$

$$B = \begin{pmatrix} -62.623 & 80.052 & -25.737 & 13.188 & -7.99 & 4.976 & -1.865 \\ 22.579 & -82.222 & 75.799 & -23.892 & 12.242 & -7.102 & 2.597 \\ -3.984 & 41.6 & -109.319 & 90.627 & -27.8 & 13.572 & -4.695 \\ 1.583 & -10.166 & 70.264 & -166.993 & 132.723 & -39.386 & 11.975 \\ -0.986 & 5.358 & -22.169 & 136.515 & -322.494 & 255.954 & -52.178 \\ 0.905 & -4.578 & 15.942 & -59.671 & 377.009 & -1.024 \times 10^{3} & 694.743 \\ 46.257 & -195.81 & 488.506 & -1.025 \times 10^{3} & 2.045 \times 10^{3} & -3.127 \times 10^{3} & 1.768 \times 10^{3} \end{pmatrix}$$