NAG Library Function Document

nag_1d_cheb_deriv (e02ahc)

1 Purpose

nag_1d_cheb_deriv (e02ahc) determines the coefficients in the Chebyshev series representation of the derivative of a polynomial given in Chebyshev series form.

2 Specification

```c
#include <nag.h>
#include <nage02.h>

void nag_1d_cheb_deriv (Integer n, double xmin, double xmax,
                       const double a[], Integer ia1, double *patm1, double adif[],
                       Integer iadif1, NagError *fail)
```

3 Description

nag_1d_cheb_deriv (e02ahc) forms the polynomial which is the derivative of a given polynomial. Both the original polynomial and its derivative are represented in Chebyshev series form. Given the coefficients $a_i$, for $i = 0, 1, \ldots, n$, of a polynomial $p(x)$ of degree $n$, where

$$p(x) = \frac{1}{2}a_0 + a_1 T_1(x) + \cdots + a_n T_n(x)$$

the function returns the coefficients $\bar{a}_i$, for $i = 0, 1, \ldots, n - 1$, of the polynomial $q(x)$ of degree $n - 1$, where

$$q(x) = \frac{dp(x)}{dx} = \frac{1}{2} \bar{a}_0 + \bar{a}_1 T_1(x) + \cdots + \bar{a}_{n-1} T_{n-1}(x).$$

Here $T_j(\bar{x})$ denotes the Chebyshev polynomial of the first kind of degree $j$ with argument $\bar{x}$. It is assumed that the normalized variable $\bar{x}$ in the interval $[-1,1]$ was obtained from your original variable $x$ in the interval $[x_{\text{min}}, x_{\text{max}}]$ by the linear transformation

$$\bar{x} = \frac{2x - (x_{\text{max}} + x_{\text{min}})}{x_{\text{max}} - x_{\text{min}}}$$

and that you require the derivative to be with respect to the variable $x$. If the derivative with respect to $\bar{x}$ is required, set $x_{\text{max}} = 1$ and $x_{\text{min}} = -1$.

Values of the derivative can subsequently be computed, from the coefficients obtained, by using nag_1d_cheb_eval2 (e02akc).

The method employed is that of Chebyshev series (see Chapter 8 of Modern Computing Methods (1961)), modified to obtain the derivative with respect to $x$. Initially setting $\bar{a}_{n+1} = \bar{a}_n = 0$, the function forms successively

$$\bar{a}_{i-1} = \bar{a}_{i+1} + \frac{2}{x_{\text{max}} - x_{\text{min}}} 2i a_i, \quad i = n, n - 1, \ldots, 1.$$

4 References

5 Arguments

1: \( n \) – Integer \( \text{Input} \)
   
   On entry: \( n \), the degree of the given polynomial \( p(x) \).
   
   Constraint: \( n \geq 0 \).

2: \( x_{\text{min}} \) – double \( \text{Input} \)

3: \( x_{\text{max}} \) – double \( \text{Input} \)

   On entry: the lower and upper end points respectively of the interval \([x_{\text{min}}, x_{\text{max}}]\). The Chebyshev series representation is in terms of the normalized variable \( \bar{x} \), where
   \[
   \bar{x} = \frac{2x - (x_{\text{max}} + x_{\text{min}})}{x_{\text{max}} - x_{\text{min}}}.
   \]

   Constraint: \( x_{\text{max}} > x_{\text{min}} \).

4: \( a[\text{dim}] \) – const double \( \text{Input} \)

   Note: the dimension, \( \text{dim} \), of the array \( a \) must be at least \((1 + (n + 1 - 1) \times \text{ia1})\).

   On entry: the Chebyshev coefficients of the polynomial \( p(x) \). Specifically, element \( i \times \text{ia1} \) of \( a \) must contain the coefficient \( a_i \), for \( i = 0, 1, \ldots, n \). Only these \( n + 1 \) elements will be accessed.

5: \( \text{ia1} \) – Integer \( \text{Input} \)

   On entry: the index increment of \( a \). Most frequently the Chebyshev coefficients are stored in adjacent elements of \( a \), and \( \text{ia1} \) must be set to 1. However, if for example, they are stored in \( a[0], a[3], a[6], \ldots \), then the value of \( \text{ia1} \) must be 3. See also Section 9.

   Constraint: \( \text{ia1} \geq 1 \).

6: \( \text{patm1} \) – double * \( \text{Output} \)

   On exit: the value of \( p(x_{\text{min}}) \). If this value is passed to the integration function nag_1d_cheb_intg (e02ajc) with the coefficients of \( q(x) \), then the original polynomial \( p(x) \) is recovered, including its constant coefficient.

7: \( \text{adif}[\text{dim}] \) – double \( \text{Output} \)

   Note: the dimension, \( \text{dim} \), of the array \( \text{adif} \) must be at least \((1 + (n + 1 - 1) \times \text{iadif1})\).

   On exit: the Chebyshev coefficients of the derived polynomial \( q(x) \). (The differentiation is with respect to the variable \( x \).) Specifically, element \( i \times \text{iadif1} \) of \( \text{adif} \) contains the coefficient \( \hat{a}_i \), for \( i = 0, 1, \ldots, n - 1 \). Additionally, element \( n \times \text{iadif1} \) is set to zero.

8: \( \text{iadif1} \) – Integer \( \text{Input} \)

   On entry: the index increment of \( \text{adif} \). Most frequently the Chebyshev coefficients are required in adjacent elements of \( \text{adif} \), and \( \text{iadif1} \) must be set to 1. However, if, for example, they are to be stored in \( \text{adif}[0], \text{adif}[3], \text{adif}[6], \ldots \), then the value of \( \text{iadif1} \) must be 3. See Section 9.

   Constraint: \( \text{iadif1} \geq 1 \).

9: \( \text{fail} \) – NagError * \( \text{Input/Output} \)

   The NAG error argument (see Section 3.6 in the Essential Introduction).
6 Error Indicators and Warnings

NE_ALLOC_FAIL
  Dynamic memory allocation failed.
  See Section 3.2.1.2 in the Essential Introduction for further information.

NE_BAD_PARAM
  On entry, argument ⟨value⟩ had an illegal value.

NE_INT
  On entry, ia1 = ⟨value⟩.
  Constraint: ia1 ≥ 1.
  On entry, iadif1 = ⟨value⟩.
  Constraint: iadif1 ≥ 1.
  On entry, n + 1 = ⟨value⟩.
  Constraint: n + 1 ≥ 1.
  On entry, n = ⟨value⟩.
  Constraint: n ≥ 0.

NE_INTERNAL_ERROR
  An internal error has occurred in this function. Check the function call and any array sizes. If the
  call is correct then please contact NAG for assistance.
  An unexpected error has been triggered by this function. Please contact NAG.
  See Section 3.6.6 in the Essential Introduction for further information.

NE_NO_LICENCE
  Your licence key may have expired or may not have been installed correctly.
  See Section 3.6.5 in the Essential Introduction for further information.

NE_REAL_2
  On entry, xmax = ⟨value⟩ and xmin = ⟨value⟩.
  Constraint: xmax > xmin.

7 Accuracy
There is always a loss of precision in numerical differentiation, in this case associated with the
multiplication by 2i in the formula quoted in Section 3.

8 Parallelism and Performance
Not applicable.

9 Further Comments
The time taken is approximately proportional to n + 1.

The increments ia1, iadif1 are included as arguments to give a degree of flexibility which, for example,
allows a polynomial in two variables to be differentiated with respect to either variable without
rearranging the coefficients.
10 Example

Suppose a polynomial has been computed in Chebyshev series form to fit data over the interval 
$[-0.5, 2.5]$. The following program evaluates the first and second derivatives of this polynomial at 4 
equally spaced points over the interval. (For the purposes of this example, $x_{\text{min}}$, $x_{\text{max}}$ and the 
Chebyshev coefficients are simply supplied. Normally a program would first read in or generate data 
and compute the fitted polynomial.)

10.1 Program Text

/* nag_1d_cheb_deriv (e02ahc) Example Program. 
* Copyright 2014 Numerical Algorithms Group. 
* Mark 7, 2001. */

#include <stdio.h>
#include <nag.h>
#include <nag_stdlib.h>
#include <nage02.h>

int main(void)
{
    const double xmin = -0.5;
    const double xmax = 2.5;
    const double a[7] =
      { 2.53213, 1.13032, 0.2715, 0.04434, 0.00547, 5.4e-4, 4e-5 };nag_1d_cheb_deriv(n, xmin, xmax, a, one, &patm1, adif, one, &fail);
    if (fail.code != NE_NOERROR)
    {
        printf("Error from nag_1d_cheb_deriv (e02ahc) call 1.\n%s\n", fail.message);
        goto END;
    }
    printf("nag_1d_cheb_deriv (e02ahc) Example Program Results\n");
    n = 6;
    one = 1;
    if (!adif || !adif2)
    {
        printf("Allocation failure\n");
        exit_status = -1;
        goto END;
    }
    println("nag_1d_cheb_deriv (e02ahc). 
* Derivative of fitted polynomial in Chebyshev series form 
*/
    nag_1d_cheb_deriv(n, xmin, xmax, a, one, &patm1, adif, one, &fail);
    if (fail.code != NE_NOERROR)
    {
        printf("Error from nag_1d_cheb_deriv (e02ahc) call 1.\n%s\n", fail.message);
        exit_status = 1;
        goto END;
    }
    println("nag_1d_cheb_deriv (e02ahc), see above. */
    nag_1d_cheb_deriv(n, xmin, xmax, adif, one, &patm1, adif2, one, &fail);
if (fail.code != NE_NOERROR)
{
    printf("Error from nag_1d_cheb_deriv (e02ahc) call 2.\n%s\n", fail.message);
    exit_status = 1;
    goto END;
}

m = 4;
printf("\n");
printf(" i Argument 1st deriv 2nd deriv\n");
for (i = 1; i <= m; ++i)
{
    x = (xmin * (double)(m - i) + xmax * (double)(i - 1)) / (double)(m - 1);
    /* nag_1d_cheb_eval2 (e02akc).
    * Evaluation of fitted polynomial in one variable from
    * Chebyshev series form
    * /
    nag_1d_cheb_eval2(n, xmin, xmax, adif, one, x, &deriv, &fail);
    if (fail.code != NE_NOERROR)
    {
        printf("Error from nag_1d_cheb_eval2 (e02akc) call 1.\n%s\n", fail.message);
        exit_status = 1;
        goto END;
    }
    /* nag_1d_cheb_eval2 (e02akc), see above. */
    nag_1d_cheb_eval2(n, xmin, xmax, adif2, one, x, &deriv2, &fail);
    if (fail.code != NE_NOERROR)
    {
        printf("Error from nag_1d_cheb_eval2 (e02akc) call 2.\n%s\n", fail.message);
        exit_status = 1;
        goto END;
    }
    printf("%4"NAG_IFMT"%9.4f %9.4f %9.4f \n", i, x, deriv, deriv2);
}

END:
NAG_FREE(adif);
NAG_FREE(adif2);

return exit_status;

10.2 Program Data

None.

10.3 Program Results

nag_1d_cheb_deriv (e02ahc) Example Program Results

<table>
<thead>
<tr>
<th>i</th>
<th>Argument</th>
<th>1st deriv</th>
<th>2nd deriv</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-0.5000</td>
<td>0.2453</td>
<td>0.1637</td>
</tr>
<tr>
<td>2</td>
<td>0.5000</td>
<td>0.4777</td>
<td>0.3185</td>
</tr>
<tr>
<td>3</td>
<td>1.5000</td>
<td>0.9304</td>
<td>0.6203</td>
</tr>
<tr>
<td>4</td>
<td>2.5000</td>
<td>1.8119</td>
<td>1.2056</td>
</tr>
</tbody>
</table>
Example Program
Evaluation of Chebyshev Polynomial and its Derivatives