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GALAHAD

ROOTS

USER DOCUMENTATION

GALAHAD Optimization Library version 5.0

1 SUMMARY

This package uses classical formulae together with Newton's method to find all the real roots of a real polynomial.

ATTRIBUTES — Versions: GALAHAD_ROOTS_single, GALAHAD_ROOTS_double. **Uses:** GALAHAD_SYMBOLS, GALAHAD_SPACE, GALAHAD_SPECFILE, GALAHAD_SORT. **Date:** November 2010. **Origin:** N. I. M. Gould, Rutherford Appleton Laboratory. **Language:** Fortran 95 + TR 15581 or Fortran 2003.

2 HOW TO USE THE PACKAGE

The package is available using both single and double precision reals, and either 32-bit or 64-bit integers. Access to the 32-bit integer, single precision version requires the `USE` statement

```
USE GALAHAD_ROOTS_single
```

with the obvious substitution `GALAHAD_ROOTS_double`, `GALAHAD_ROOTS_single_64` and `GALAHAD_ROOTS_double_64` for the other variants.

If it is required to use more than one of the modules at the same time, the derived types `ROOTS_control_type`, `ROOTS_inform_type` and `ROOTS_data_type` (Section 2.2) and the subroutine `ROOTS_solve`, (Section 2.3) must be renamed on one of the `USE` statements.

2.1 Real and integer kinds

We use the terms integer and real to refer to the fortran keywords `REAL(rp_)` and `INTEGER(ip_)`, where `rp_` and `ip_` are the relevant kind values for the real and integer types employed by the particular module in use. The former are equivalent to default `REAL` for the single precision versions and `DOUBLE PRECISION` for the double precision cases, and correspond to `rp_ = real32` and `rp_ = real64`, respectively, as supplied by the fortran `iso_fortran_env` module. The latter are default (32-bit) and long (64-bit) integers, and correspond to `ip_ = int32` and `ip_ = int64`, respectively, again from the `iso_fortran_env` module.

2.2 The derived data types

Three derived data types are accessible from the package.

2.2.1 The derived data type for holding control parameters

The derived data type `ROOTS_control_type` is used to hold controlling data. Default values may be obtained by calling `ROOTS_initialize` (see Section 2.3.1), while components may also be changed by calling `ROOTS_read_specfile` (see Section 2.5.1). The components of `ROOTS_control_type` are:

`error` is a scalar variable of type `INTEGER(ip_)`, that holds the stream number for error messages. Printing of error messages in `ROOTS_solve` and `ROOTS_terminate` is suppressed if `error ≤ 0`. The default is `error = 6`.

`out` is a scalar variable of type `INTEGER(ip_)`, that holds the stream number for informational messages. Printing of informational messages in `ROOTS_solve` is suppressed if `out < 0`. The default is `out = 6`.

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`print_level` is a scalar variable of type `INTEGER(ip_)`, that is used to control the amount of informational output which is required. No informational output will occur if `print_level ≤ 0`. If `print_level ≥ 1`, debugging information will be provided. The default is `print_level = 0`.

`tol` is an `INTENT(IN)` scalar of type `REAL(rp_)` that should be set to the required accuracy of the roots. Every effort will be taken to ensure that each computed root x_c lies within $\pm \text{tol } x_e$ of its exact equivalent x_e , although sometimes the required accuracy will not be possible. The default is `tol = EPSILON(1.0)` (`EPSILON(1.0D0)` in `GALAHAD_ROOTS_double`).

`space_critical` is a scalar variable of type default `LOGICAL`, that must be set `.TRUE.` if space is critical when allocating arrays and `.FALSE.` otherwise. The package may run faster if `space_critical` is `.FALSE.` but at the possible expense of a larger storage requirement. The default is `space_critical = .FALSE..`

`deallocate_error_fatal` is a scalar variable of type default `LOGICAL`, that must be set `.TRUE.` if the user wishes to terminate execution if a deallocation fails, and `.FALSE.` if an attempt to continue will be made. The default is `deallocate_error_fatal = .FALSE..`

`prefix` is a scalar variable of type default `CHARACTER` and length 30, that may be used to provide a user-selected character string to preface every line of printed output. Specifically, each line of output will be prefaced by the string `prefix(2:LEN(TRIM(prefix))-1)`, thus ignoring the first and last non-null components of the supplied string. If the user does not want to preface lines by such a string, they may use the default `prefix = ""`.

2.2.2 The derived data type for holding informational parameters

The derived data type `ROOTS_inform_type` is used to hold parameters that give information about the progress and needs of the algorithm. The components of `ROOTS_inform_type` are:

`status` is a scalar variable of type `INTEGER(ip_)`, that gives the exit status of the algorithm. See Section 2.4 for details.

`alloc_status` is a scalar variable of type `INTEGER(ip_)`, that gives the status of the last attempted array allocation or deallocation. This will be 0 if `status = 0`.

`bad_alloc` is a scalar variable of type default `CHARACTER` and length 80, that gives the name of the last internal array for which there were allocation or deallocation errors. This will be the null string if `status = 0`.

2.2.3 The derived data type for holding problem data

The derived data type `ROOTS_data_type` is used to hold all the data for a particular problem, between calls of `ROOTS` procedures. This data should be preserved, untouched, from the initial call to `ROOTS_initialize` to the final call to `ROOTS_terminate`.

2.3 Argument lists and calling sequences

There are three procedures for user calls (see Section 2.5 for further features):

1. The subroutine `ROOTS_initialize` is used to set default values, and initialize private data.
2. The subroutine `ROOTS_solve` is called to find the real roots of the polynomial

$$\sum_{i=0}^d a_i x^i \tag{2.1}$$

of degree d , where the coefficients a_i , $0 \leq i \leq d$ are real.

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3. The subroutine `ROOTS_terminate` allows the user to automatically deallocate array components of the private data, allocated by `ROOTS_solve`, at the end of the solution process.

2.3.1 The initialization subroutine

Default values are provided as follows:

```
CALL ROOTS_initialize( data, control, inform )
```

`data` is a scalar `INTENT(INOUT)` argument of type `ROOTS_data_type` (see Section 2.2.3). It is used to hold data about the problem being solved.

`control` is a scalar `INTENT(OUT)` argument of type `ROOTS_control_type` (see Section 2.2.1). On exit, `control` contains default values for the components as described in Section 2.2.1. These values should only be changed after calling `ROOTS_initialize`.

`inform` is a scalar `INTENT(OUT)` argument of type `ROOTS_inform_type` (see Section 2.2.2). A successful call to `ROOTS_initialize` is indicated when the component status has the value 0.

2.3.2 The solution subroutine

The roots of the polynomial (2.1) are found as follows

```
CALL ROOTS_solve( A, nroots, ROOTS, control, inform, data )
```

`A` is an `INTENT(IN)` rank-one array of type `REAL(rp_)`, whose lower bound must be 0 and whose upper bound specifies the degree, d , of the polynomial. The entries $A(i), i = 0, \dots, \text{UBOUND}(A)$, must contain the values of the real coefficients $a_i, 0 \leq i \leq d$. **Restrictions:** $\text{UBOUND}(A, 1) \geq 0$.

`nroots` is an `INTENT(OUT)` scalar of type `INTEGER(ip_)`, that gives the number of real roots of the polynomial.

`ROOTS` is an `INTENT(OUT)` rank-one array of length d and type `REAL(rp_)`. On exit, `ROOTS(:nroots)` give the values of the real roots of the polynomial in increasing order. **Restrictions:** $\text{SIZE}(\text{ROOTS}) \geq \text{UBOUND}(A, 1)$.

`control` is a scalar `INTENT(IN)` argument of type `ROOTS_control_type` (see Section 2.2.1). Default values may be assigned by calling `ROOTS_initialize` prior to the first call to `ROOTS_solve`.

`inform` is a scalar `INTENT(INOUT)` argument of type `ROOTS_inform_type` (see Section 2.2.2). A successful call to `ROOTS_solve` is indicated when the component status has the value 0. For other return values of status, see Section 2.4.

`data` is a scalar `INTENT(INOUT)` argument of type `ROOTS_data_type` (see Section 2.2.3). It is used to hold data about the problem being solved. It must not have been altered by the user since the last call to `ROOTS_initialize`.

2.3.3 The termination subroutine

All previously allocated arrays are deallocated as follows:

```
CALL ROOTS_terminate( data, control, inform )
```

`data` is a scalar `INTENT(INOUT)` argument of type `ROOTS_data_type` exactly as for `ROOTS_solve`, which must not have been altered by the user since the last call to `ROOTS_initialize`. On exit, array components will have been deallocated.

`control` is a scalar `INTENT(IN)` argument of type `ROOTS_control_type` exactly as for `ROOTS_solve`.

`inform` is a scalar `INTENT(OUT)` argument of type `ROOTS_inform_type` exactly as for `ROOTS_solve`. Only the component status will be set on exit, and a successful call to `ROOTS_terminate` is indicated when this component status has the value 0. For other return values of status, see Section 2.4.

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2.4 Warning and error messages

A negative value of `inform%status` on exit from `ROOTS_solve` indicates that an error has occurred. No further calls should be made until the error has been corrected. Possible values are:

- 1. An allocation error occurred. A message indicating the offending array is written on unit `control%error`, and the returned allocation status and a string containing the name of the offending array are held in `inform%alloc_status` and `inform%bad_alloc` respectively.
- 2. A deallocation error occurred. A message indicating the offending array is written on unit `control%error` and the returned allocation status and a string containing the name of the offending array are held in `inform%alloc_status` and `inform%bad_alloc` respectively.
- 3. Either the specified degree of the polynomial in `degree` is less than 0, or the declared dimension of the array `ROOTS` is smaller than the specified degree.

2.5 Further features

In this section, we describe an alternative means of setting control parameters, that is components of the variable `control` of type `ROOTS_control_type` (see Section 2.2.1), by reading an appropriate data specification file using the subroutine `ROOTS_read_specfile`. This facility is useful as it allows a user to change `ROOTS` control parameters without editing and recompiling programs that call `ROOTS`.

A specification file, or `specfile`, is a data file containing a number of "specification commands". Each command occurs on a separate line, and comprises a "keyword", which is a string (in a close-to-natural language) used to identify a control parameter, and an (optional) "value", which defines the value to be assigned to the given control parameter. All keywords and values are case insensitive, keywords may be preceded by one or more blanks but values must not contain blanks, and each value must be separated from its keyword by at least one blank. Values must not contain more than 30 characters, and each line of the `specfile` is limited to 80 characters, including the blanks separating keyword and value.

The portion of the specification file used by `ROOTS_read_specfile` must start with a "BEGIN ROOTS" command and end with an "END" command. The syntax of the `specfile` is thus defined as follows:

```
( .. lines ignored by CQP_read_specfile .. )
BEGIN CQP
  keyword    value
  .....     .....
  keyword    value
END
( .. lines ignored by CQP_read_specfile .. )
```

where `keyword` and `value` are two strings separated by (at least) one blank. The "BEGIN ROOTS" and "END" delimiter command lines may contain additional (trailing) strings so long as such strings are separated by one or more blanks, so that lines such as

```
BEGIN CQP SPECIFICATION
```

and

```
END CQP SPECIFICATION
```

are acceptable. Furthermore, between the "BEGIN ROOTS" and "END" delimiters, specification commands may occur in any order. Blank lines and lines whose first non-blank character is `!` or `*` are ignored. The content of a line after a `!`

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or * character is also ignored (as is the ! or * character itself). This provides an easy manner to "comment out" some specification commands, or to comment specific values of certain control parameters.

The value of a control parameters may be of three different types, namely integer, logical or real. Integer and real values may be expressed in any relevant Fortran integer and floating-point formats (respectively). Permitted values for logical parameters are "ON", "TRUE", ".TRUE.", "T", "YES", "Y", or "OFF", "NO", "N", "FALSE", ".FALSE." and "F". Empty values are also allowed for logical control parameters, and are interpreted as "TRUE".

The specification file must be open for input when `ROOTS_read_specfile` is called, and the associated device number passed to the routine in `device` (see below). Note that the corresponding file is `REWINDED`, which makes it possible to combine the specifications for more than one program/routine. For the same reason, the file is not closed by `ROOTS_read_specfile`.

2.5.1 To read control parameters from a specification file

Control parameters may be read from a file as follows:

```
CALL CQP_read_specfile( control, device )
```

`control` is a scalar `INTENT(INOUT)` argument of type `ROOTS_control_type` (see Section 2.2.1). Default values should have already been set, perhaps by calling `ROOTS_initialize`. On exit, individual components of `control` may have been changed according to the commands found in the specfile. Specfile commands and the component (see Section 2.2.1) of `control` that each affects are given in Table 2.1.

command	component of control	value type
error-printout-device	%error	integer
printout-device	%out	integer
print-level	%print_level	integer
root-tolerance	%tol	real
space-critical	%space_critical	logical
deallocate-error-fatal	%deallocate_error_fatal	logical
output-line-prefix	%prefix	character

Table 2.1: Specfile commands and associated components of `control`.

`device` is a scalar `INTENT(IN)` argument of type `INTEGER(ip_)`, that must be set to the unit number on which the specfile has been opened. If `device` is not open, `control` will not be altered and execution will continue, but an error message will be printed on unit `control%error`.

3 GENERAL INFORMATION

Use of common: None.

Workspace: Provided automatically by the module.

Other routines called directly: None.

Other modules used directly: `ROOTS_solve` calls the GALAHAD packages `GALAHAD_SYMBOLS`, `GALAHAD_SPACE`, `GALAHAD_SPECFILE` and `GALAHAD_SORT`.

Input/output: Output is under control of the arguments `control%error`, `control%out` and `control%print_level`.

Portability: ISO Fortran 95 + TR 15581 or Fortran 2003. The package is thread-safe.

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4 METHOD

Littlewood and Ferrari's algorithms are used to find estimates of the real roots of cubic and quartic polynomials, respectively; a stabilized version of the well-known formula is used in the quadratic case. Newton's method and/or methods based on the companion matrix are used to further refine the computed roots if necessary. Madsen and Reid's (1975) method is used for polynomials whose degree exceeds four.

References:

The basic method is that given by

K. Madsen and J. K. Reid, "FORTRAN Subroutines for Finding Polynomial Zeros". Technical Report A.E.R.E. R.7986, Computer Science and System Division, A.E.R.E. Harwell, Oxfordshire, U.K. (1975)

5 EXAMPLE OF USE

Suppose we wish to solve the quadratic, cubic, quartic and quintic equations

$$\begin{aligned}x^2 - 3x + 2 &= 0 \\x^3 - 6x^2 + 11x - 6 &= 0 \\x^4 - 10x^3 + 35x^2 - 50x + 24 &= 0 \text{ and} \\x^5 - 15x^4 + 85x^3 - 225x^2 + 274x - 120 &= 0.\end{aligned}$$

Then we may use the following code:

```
! THIS VERSION: GALAHAD 2.1 - 22/03/2007 AT 09:00 GMT.
PROGRAM GALAHAD_ROOTS_EXAMPLE
USE GALAHAD_ROOTS_double      ! double precision version
IMPLICIT NONE
INTEGER, PARAMETER :: wp = KIND( 1.0D+0 ) ! set precision
REAL ( KIND = wp ), PARAMETER :: one = 1.0_wp
INTEGER :: degree, nroots
REAL ( KIND = wp ) :: A( 0 : 5 ), ROOTS( 5 )
TYPE ( ROOTS_data_type ) :: data
TYPE ( ROOTS_control_type ) :: control
TYPE ( ROOTS_inform_type ) :: inform
control%tol = EPSILON( one ) ** 0.75      ! accuracy requested
DO degree = 2, 5                          ! polynomials of degree 2 to 5
  IF ( degree == 2 ) THEN
    A( 0 ) = 2.0_wp
    A( 1 ) = - 3.0_wp
    A( 2 ) = 1.0_wp
    WRITE( 6, "( ' Quadratic ' )" )
    CALL ROOTS_solve( A( : degree ), nroots, ROOTS( : degree ),
                     control, inform, data )
  ELSE IF ( degree == 3 ) THEN
    A( 0 ) = - 6.0_wp
    A( 1 ) = 11.0_wp
    A( 2 ) = - 6.0_wp
    A( 3 ) = 1.0_wp
    WRITE( 6, "( /, ' Cubic ' )" )
    CALL ROOTS_solve( A( : degree ), nroots, ROOTS( : degree ),
                     control, inform, data )
  ELSE IF ( degree == 4 ) THEN
```

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```

A( 0 ) = 24.0_wp
A( 1 ) = - 50.0_wp
A( 2 ) = 35.0_wp
A( 3 ) = - 10.0_wp
A( 4 ) = 1.0_wp
WRITE( 6, "( /, ' Quartic ' )" )
CALL ROOTS_solve( A( : degree ), nroots, ROOTS( : degree ),      &
                 control, inform, data )
ELSE IF ( degree == 5 ) THEN
A( 0 ) = - 120.0_wp
A( 1 ) = 274.0_wp
A( 2 ) = - 225.0_wp
A( 3 ) = 85.0_wp
A( 4 ) = - 15.0_wp
A( 5 ) = 1.0_wp
WRITE( 6, "( /, ' Quintic ' )" )
CALL ROOTS_solve( A( : degree ), nroots, ROOTS( : degree ),      &
                 control, inform, data )
END IF
IF ( nroots == 0 ) THEN
WRITE( 6, "( ' no real roots ' )" )
ELSE IF ( nroots == 1 ) THEN
WRITE( 6, "( ' 1 real root ' )" )
ELSE IF ( nroots == 2 ) THEN
WRITE( 6, "( ' 2 real roots ' )" )
ELSE IF ( nroots == 3 ) THEN
WRITE( 6, "( ' 3 real roots ' )" )
ELSE IF ( nroots == 4 ) THEN
WRITE( 6, "( ' 4 real roots ' )" )
ELSE IF ( nroots == 5 ) THEN
WRITE( 6, "( ' 5 real roots ' )" )
END IF
IF ( nroots /= 0 ) WRITE( 6, "( ' roots: ', 5ES10.2 )" ) ROOTS( : nroots )
END DO
END PROGRAM GALAHAD_ROOTS_EXAMPLE

```

This produces the following output:

```

Quadratic
2 real roots
roots:  1.00E+00  2.00E+00

Cubic
3 real roots
roots:  1.00E+00  2.00E+00  3.00E+00

Quartic
4 real roots
roots:  1.00E+00  2.00E+00  3.00E+00  4.00E+00

Quintic
5 real roots
roots:  1.00E+00  2.00E+00  3.00E+00  4.00E+00  5.00E+00

```

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