NAG Library Function Document

nag_sum_fft_real_3d (c06pyc)

1 Purpose

nag_sum_fft_real_3d (c06pyc) computes the three-dimensional discrete Fourier transform of a trivariate sequence of real data values.

2 Specification

```
#include <nag.h>
#include <nagc06.h>
```

```
void nag_sum_fft_real_3d (Integer n1, Integer n2, Integer n3,
     const double x[], Complex y[], NagError *fail)
```

3 Description

nag_sum_fft_real_3d (c06pyc) computes the three-dimensional discrete Fourier transform of a trivariate sequence of real data values $x_{j_1j_2j_3}$, for $j_1 = 0,1,\ldots,n_1-1$, $j_2 = 0,1,\ldots,n_2-1$ and $j_3 = 0,1,\ldots,n_3-1$.

The discrete Fourier transform is here defined by

$$\hat{z}_{k_1k_2k_3} = \frac{1}{\sqrt{n_1n_2n_3}}\sum_{j_1=0}^{n_1-1}\sum_{j_2=0}^{n_2-1}\sum_{j_3=0}^{n_3-1}x_{j_1j_2j_3} \times \exp\left(-2\pi i\left(\frac{j_1k_1}{n_1}+\frac{j_2k_2}{n_2}+\frac{j_3k_3}{n_3}\right)\right),$$

where $k_1 = 0,1,\ldots,n_1-1$, $k_2 = 0,1,\ldots,n_2-1$ and $k_3 = 0,1,\ldots,n_3-1$. (Note the scale factor of $\frac{1}{\sqrt{n_1n_2n_3}}$ in this definition.)

The transformed values $\hat{z}_{k_1k_2k_3}$ are complex. Because of conjugate symmetry (i.e., $\hat{z}_{k_1k_2k_3}$ is the complex conjugate of $\hat{z}_{(n_1-k_1)k_2k_3}$), only slightly more than half of the Fourier coefficients need to be stored in the output.

A call of nag_sum_fft_real_3d (c06pyc) followed by a call of nag_sum_fft_hermitian_3d (c06pzc) will restore the original data.

This function performs multiple one-dimensional discrete Fourier transforms by the fast Fourier transform (FFT) algorithm in Brigham (1974) and Temperton (1983).

4 References

Brigham E O (1974) *The Fast Fourier Transform* Prentice–Hall

Temperton C (1983) Fast mixed-radix real Fourier transforms *J. Comput. Phys.* **52** 340–350

5 Arguments

1: **n1** – Integer *Input*

On entry: n_1, the first dimension of the transform.

Constraint: $\mathbf{n1} \geq 1$.

2: **n2** – Integer *Input*

On entry: n_2, the second dimension of the transform.

Constraint: $\mathbf{n2} \geq 1$.

3: **n3** – Integer *Input*

On entry: n_3, the third dimension of the transform.

Constraint: **n3** ≥ 1.

4: **x**[**n1** $\times$ **n2** $\times$ **n3**] – const double *Input*

On entry: the real input dataset x, where $x_{j_1 j_2 j_3}$ is stored in **x**[$j_3 \times n_1 n_2 + j_2 \times n_1 + j_1$], for $j_1 = 0, 1, \ldots, n_1 - 1$, $j_2 = 0, 1, \ldots, n_2 - 1$ and $j_3 = 0, 1, \ldots, n_3 - 1$.

5: **y**[*dim*] – Complex *Output*

Note: the dimension, *dim*, of the array **y** must be at least $(\mathbf{n1}/2 + 1) \times \mathbf{n2} \times \mathbf{n3}$.

On exit: the complex output dataset $\hat{z}$, where $\hat{z}_{k_1 k_2 k_3}$ is stored in **y**[$k_3 \times (n_1/2 + 1)n_2 + k_2 \times (n_1/2 + 1) + k_1$], for $k_1 = 0, 1, \ldots, n_1/2$, $k_2 = 0, 1, \ldots, n_2 - 1$ and $k_3 = 0, 1, \ldots, n_3 - 1$. Note the first dimension is cut roughly by half to remove the redundant information due to conjugate symmetry.

6: **fail** – NagError * *Input/Output*

The NAG error argument (see Section 2.7 in How to Use the NAG Library and its Documentation).

6 Error Indicators and Warnings

NE_ALLOC_FAIL

Dynamic memory allocation failed.
See Section 2.3.1.2 in How to Use the NAG Library and its Documentation for further information.

NE_BAD_PARAM

On entry, argument $\langle$*value*$\rangle$ had an illegal value.

NE_INT

On entry, **n1** $= \langle$*value*$\rangle$.
Constraint: **n1** ≥ 1.

On entry, **n2** $= \langle$*value*$\rangle$.
Constraint: **n2** ≥ 1.

On entry, **n3** $= \langle$*value*$\rangle$.
Constraint: **n3** ≥ 1.

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 2.7.6 in How to Use the NAG Library and its Documentation for further information.

NE_NO_LICENCE

Your licence key may have expired or may not have been installed correctly.
See Section 2.7.5 in How to Use the NAG Library and its Documentation for further information.

7 Accuracy

Some indication of accuracy can be obtained by performing a forward transform using nag_sum_fft_real_3d (c06pyc) and a backward transform using nag_sum_fft_hermitian_3d (c06pzc), and comparing the results with the original sequence (in exact arithmetic they would be identical).

8 Parallelism and Performance

nag_sum_fft_real_3d (c06pyc) is threaded by NAG for parallel execution in multithreaded implementations of the NAG Library.

nag_sum_fft_real_3d (c06pyc) makes calls to BLAS and/or LAPACK routines, which may be threaded within the vendor library used by this implementation. Consult the documentation for the vendor library for further information.

Please consult the x06 Chapter Introduction for information on how to control and interrogate the OpenMP environment used within this function. Please also consult the Users' Note for your implementation for any additional implementation-specific information.

9 Further Comments

The time taken by nag_sum_fft_real_3d (c06pyc) is approximately proportional to $n_1n_2n_3\log(n_1n_2n_3)$, but also depends on the factors of n_1, n_2 and n_3. nag_sum_fft_real_3d (c06pyc) is fastest if the only prime factors of n_1, n_2 and n_3 are 2, 3 and 5, and is particularly slow if one of the dimensions is a large prime, or has large prime factors.

Workspace is internally allocated by nag_sum_fft_real_3d (c06pyc). The total size of these arrays is approximately proportional to $n_1n_2n_3$.

10 Example

This example reads in a trivariate sequence of real data values and prints their discrete Fourier transforms as computed by nag_sum_fft_real_3d (c06pyc). Inverse transforms are then calculated by calling nag_sum_fft_hermitian_3d (c06pzc) showing that the original sequences are restored.

10.1 Program Text

```
/* nag_sum_fft_real_3d (c06pyc) Example Program.
 *
 * NAGPRODCODE Version.
 *
 * Copyright 2016 Numerical Algorithms Group.
 *
 * Mark 26, 2016.
 */

#include <stdio.h>
#include <nag.h>
#include <nag_stdlib.h>
#include <nagc06.h>

int main(void)
{
  /* Scalars */
  Integer exit_status = 0, k, n1, n2, n3;
  /* Arrays */
  Complex *y = 0;
  double *x = 0;
  char title[30];
  /* Nag Types */
  NagError fail;

  INIT_FAIL(fail);
  printf("nag_sum_fft_real_3d (c06pyc) Example Program Results\n");
  fflush(stdout);

  /* Read dimensions of array from data file. */
#ifdef _WIN32
  scanf_s("%*[^\n] %" NAG_IFMT "%" NAG_IFMT "%" NAG_IFMT "%*[^\n]", &n1, &n2,
          &n3);
#else
  scanf("%*[^\n] %" NAG_IFMT "%" NAG_IFMT "%" NAG_IFMT "%*[^\n]", &n1, &n2,
        &n3);
#endif

  if (!(x = NAG_ALLOC(n1 * n2 * n3, double)) ||
      !(y = NAG_ALLOC((n1 / 2 + 1) * n2 * n3, Complex)))
  {
    printf("Allocation failure\n");
    exit_status = -1;
    goto END;
  }

  /* Read array values from data file and print out. */
  for (k = 0; k < n1 * n2 * n3; k++)
#ifdef _WIN32
    scanf_s("%lf", &x[k]);
#else
    scanf("%lf", &x[k]);
#endif

  printf("\nBelow we define X(i,j,k)=x[k*n1*n2+j*n1+i]");
  printf(" where i and j are the row and column \n");
  printf("indices of the matrices printed.");
  printf(" Y is defined similarly (but having n1/2+1 rows\n");
  printf("only due to conjugate symmetry).\n");

  printf("\n Original data values\n");
  fflush(stdout);
  for (k = 0; k < n3; k++) {
#ifdef _WIN32
    sprintf_s(title, (unsigned)_countof(title),
              "\n  X(i,j,k) for k = %" NAG_IFMT, k);
#else
    sprintf(title, "\n  X(i,j,k) for k = %" NAG_IFMT, k);
#endif
    nag_gen_real_mat_print_comp(Nag_ColMajor, Nag_GeneralMatrix,
                                Nag_NonUnitDiag, n1, n2, &x[k * n1 * n2], n1,
                                "%6.3f", title, Nag_NoLabels, 0,
                                Nag_NoLabels, 0, 80, 0, 0, &fail);
  }
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_gen_real_mat_print_comp (x04cbc).\n%s\n",
           fail.message);
    exit_status = 1;
    goto END;
  }

  /* Compute three-dimensional real-to-complex discrete Fourier transform using
   * nag_sum_fft_real_3d (c06pyc) and print out.
   */
  nag_sum_fft_real_3d(n1, n2, n3, x, y, &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_sum_fft_real_3d (c06pyc).\n%s\n", fail.message);
    exit_status = 2;
    goto END;
  }

  printf("\n Components of discrete Fourier transform\n");
  fflush(stdout);
  for (k = 0; k < n3; k++) {
#ifdef _WIN32
    sprintf_s(title, (unsigned)_countof(title),
              "\n  Y(i,j,k) for k = %" NAG_IFMT, k);
#else
    sprintf(title, "\n  Y(i,j,k) for k = %" NAG_IFMT, k);
#endif
    /* nag_gen_complx_mat_print_comp (x04dbc).
     * Print complex general matrix (comprehensive) */
    nag_gen_complx_mat_print_comp(Nag_ColMajor, Nag_GeneralMatrix,
                                  Nag_NonUnitDiag, n1 / 2 + 1, n2,
                                  &y[k * (n1 / 2 + 1) * n2], n1 / 2 + 1,
                                  Nag_BracketForm, "%6.3f", title,
                                  Nag_NoLabels, 0, Nag_NoLabels, 0, 90, 0, 0,
                                  &fail);
  }
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_gen_complx_mat_print_comp (x04dbc).\n%s\n",
           fail.message);
    exit_status = 3;
    goto END;
  }

  /* Compute three-dimensional complex-to-real discrete Fourier transform using
   * nag_sum_fft_hermitian_3d (c06pzc) and print out.
   */
  nag_sum_fft_hermitian_3d(n1, n2, n3, y, x, &fail);
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_sum_fft_hermitian_3d (c06pzc).\n%s\n",
           fail.message);
    exit_status = 4;
    goto END;
  }

  printf("\n Original sequence as restored by inverse transform\n");
  fflush(stdout);
  for (k = 0; k < n3; k++) {
#ifdef _WIN32
    sprintf_s(title, (unsigned)_countof(title),
              "\n  X(i,j,k) for k = %" NAG_IFMT, k);
#else
    sprintf(title, "\n  X(i,j,k) for k = %" NAG_IFMT, k);
#endif
    /* nag_gen_real_mat_print_comp (x04cbc).
     * Print out a real matrix (comprehensive) */
    nag_gen_real_mat_print_comp(Nag_ColMajor, Nag_GeneralMatrix,
                                Nag_NonUnitDiag, n1, n2, &x[k * n1 * n2], n1,
                                "%6.3f", title, Nag_NoLabels, 0,
                                Nag_NoLabels, 0, 80, 0, 0, &fail);
  }
  if (fail.code != NE_NOERROR) {
    printf("Error from nag_gen_real_mat_print_comp (x04cbc).\n%s\n",
           fail.message);
    exit_status = 5;
    goto END;
  }

END:
  NAG_FREE(x);
  NAG_FREE(y);
  return exit_status;
}
```

10.2 Program Data

```
nag_sum_fft_real_3d (c06pyc) Example Program Data

      3         3         4     : n1, n2, n3

      1.541     0.584     0.010
      0.346     1.284     1.960
      1.754     0.855     0.089

      0.161     1.004     1.844
      1.907     1.137     0.240
      0.042     0.725     1.660

      1.989     1.408     0.452
      0.001     0.467     1.424
      1.991     1.647     0.708

      0.037     0.252     1.154
      1.915     1.834     0.987
      0.151     0.096     0.872 : x
```

10.3 Program Results

```
nag_sum_fft_real_3d (c06pyc) Example Program Results

Below we define X(i,j,k)=x[k*n1*n2+j*n1+i] where i and j are the row and column
indices of the matrices printed. Y is defined similarly (but having n1/2+1 rows
only due to conjugate symmetry).

 Original data values

  X(i,j,k) for k = 0
   1.541  0.346  1.754
   0.584  1.284  0.855
   0.010  1.960  0.089

  X(i,j,k) for k = 1
   0.161  1.907  0.042
   1.004  1.137  0.725
   1.844  0.240  1.660

  X(i,j,k) for k = 2
   1.989  0.001  1.991
   1.408  0.467  1.647
   0.452  1.424  0.708

  X(i,j,k) for k = 3
   0.037  1.915  0.151
   0.252  1.834  0.096
   1.154  0.987  0.872

 Components of discrete Fourier transform

  Y(i,j,k) for k = 0
   ( 5.755, 0.000)  (-0.268,-0.420)  (-0.268, 0.420)
   ( 0.081, 0.015)  ( 0.038, 0.198)  ( 0.067,-0.122)

  Y(i,j,k) for k = 1
   (-0.277,-0.237)  ( 0.109,-0.756)  (-0.688, 0.210)
   ( 0.060, 0.156)  (-0.275, 0.295)  ( 0.280, 0.012)

  Y(i,j,k) for k = 2
   ( 0.415, 0.000)  ( 0.175, 0.871)  ( 0.175,-0.871)
   ( 0.645,-0.478)  ( 1.585, 0.616)  (-0.113,-1.555)

  Y(i,j,k) for k = 3
   (-0.277, 0.237)  (-0.688,-0.210)  ( 0.109, 0.756)
   ( 0.047,-0.077)  ( 0.201, 0.061)  (-0.128,-0.117)

 Original sequence as restored by inverse transform

  X(i,j,k) for k = 0
   1.541  0.346  1.754
   0.584  1.284  0.855
   0.010  1.960  0.089

  X(i,j,k) for k = 1
   0.161  1.907  0.042
   1.004  1.137  0.725
   1.844  0.240  1.660
 X(i,j,k) for k = 2
  1.989  0.001  1.991
  1.408  0.467  1.647
  0.452  1.424  0.708

 X(i,j,k) for k = 3
  0.037  1.915  0.151
  0.252  1.834  0.096
  1.154  0.987  0.872
```