# NAG Library Chapter Introduction

# c06 – Fourier Transforms

## Contents

# 1 Scope of the Chapter

This chapter is concerned with the following tasks.

(a) Calculating the **discrete Fourier transform** of a sequence of real or complex data values.

(b) Calculating the **discrete convolution** or the **discrete correlation** of two sequences of real or complex data values using discrete Fourier transforms.

(c) Direct summation of orthogonal series.

# 2 Background to the Problems

## 2.1 Discrete Fourier Transforms

### 2.1.1 Complex transforms

Most of the functions in this chapter calculate the finite **discrete Fourier transform** (DFT) of a sequence of $n$ complex numbers $z_j$, for $j = 0, 1, \ldots, n-1$. The direct transform is defined by

$$\hat{z}_k = \frac{1}{\sqrt{n}} \sum_{j=0}^{n-1} z_j \exp\left(-i\frac{2\pi jk}{n}\right) \tag{1}$$

for $k = 0, 1, \ldots, n-1$. Note that equation (1) makes sense for all integral $k$ and with this extension $\hat{z}_k$ is periodic with period $n$, i.e., $\hat{z}_k = \hat{z}_{k\pm n}$, and in particular $\hat{z}_{-k} = \hat{z}_{n-k}$. Note also that the scale-factor of $\frac{1}{\sqrt{n}}$ may be omitted in the definition of the DFT, and replaced by $\frac{1}{n}$ in the definition of the inverse.

If we write $z_j = x_j + iy_j$ and $\hat{z}_k = a_k + ib_k$, then the definition of $\hat{z}_k$ may be written in terms of sines and cosines as

$$a_k = \frac{1}{\sqrt{n}} \sum_{j=0}^{n-1} \left( x_j \cos\left(\frac{2\pi jk}{n}\right) + y_j \sin\left(\frac{2\pi jk}{n}\right) \right)$$

$$b_k = \frac{1}{\sqrt{n}} \sum_{j=0}^{n-1} \left( y_j \cos\left(\frac{2\pi jk}{n}\right) - x_j \sin\left(\frac{2\pi jk}{n}\right) \right).$$

The original data values $z_j$ may conversely be recovered from the transform $\hat{z}_k$ by an **inverse discrete Fourier transform**:

$$z_j = \frac{1}{\sqrt{n}} \sum_{k=0}^{n-1} \hat{z}_k \exp\left(+i\frac{2\pi jk}{n}\right) \tag{2}$$

for $j = 0, 1, \ldots, n-1$. If we take the complex conjugate of (2), we find that the sequence $\bar{z}_j$ is the DFT of the sequence $\bar{\hat{z}}_k$. Hence the inverse DFT of the sequence $\hat{z}_k$ may be obtained by taking the complex conjugates of the $\hat{z}_k$; performing a DFT, and taking the complex conjugates of the result. (Note that the terms **forward** transform and **backward** transform are also used to mean the direct and inverse transforms respectively.)

The definition (1) of a one-dimensional transform can easily be extended to multidimensional transforms. For example, in two dimensions we have

$$\hat{z}_{k_1 k_2} = \frac{1}{\sqrt{n_1 n_2}} \sum_{j_1=0}^{n_1-1} \sum_{j_2=0}^{n_2-1} z_{j_1 j_2} \exp\left(-i\frac{2\pi j_1 k_1}{n_1}\right) \exp\left(-i\frac{2\pi j_2 k_2}{n_2}\right). \tag{3}$$

**Note:** definitions of the discrete Fourier transform vary. Sometimes (2) is used as the definition of the DFT, and (1) as the definition of the inverse.

### 2.1.2 Real transforms

If the original sequence is purely real valued, i.e., $z_j = x_j$, then

$$\hat{z}_k = a_k + ib_k = \frac{1}{\sqrt{n}}\sum_{j=0}^{n-1} x_j \exp\left(-i\frac{2\pi jk}{n}\right)$$

and $\hat{z}_{n-k}$ is the complex conjugate of $\hat{z}_k$. Thus the DFT of a real sequence is a particular type of complex sequence, called a **Hermitian** sequence, or **half-complex** or **conjugate symmetric**, with the properties

$$a_{n-k} = a_k \quad b_{n-k} = -b_k \quad b_0 = 0$$

and, if $n$ is even, $b_{n/2} = 0$.

Thus a Hermitian sequence of $n$ complex data values can be represented by only $n$, rather than $2n$, independent real values. This can obviously lead to economies in storage, with two schemes being used in this chapter. In the first (deprecated) scheme, which will be referred to as the **real storage format** for Hermitian sequences, the real parts $a_k$ for $0 \le k \le n/2$ are stored in normal order in the first $n/2+1$ locations of an array **x** of length $n$; the corresponding nonzero imaginary parts are stored in reverse order in the remaining locations of **x**. To clarify, the following two tables illustrate the storage of the real and imaginary parts of $\hat{z}_k$ for the two cases: $n$ even and $n$ odd.

If $n$ is even then the sequence has two purely real elements and is stored as follows:

| Index of **x** | 0 | 1 | 2 | ... | $n/2$ | ... | $n-2$ | $n-1$ |
|---|---|---|---|---|---|---|---|---|
| Sequence | $a_0$ | $a_1 + ib_1$ | $a_2 + ib_2$ | ... | $a_{n/2}$ | ... | $a_2 - ib_2$ | $a_1 - ib_1$ |
| Stored values | $a_0$ | $a_1$ | $a_2$ | ... | $a_{n/2}$ | ... | $b_2$ | $b_1$ |

$$\begin{aligned} \mathbf{x}[k] &= a_k, && \text{for } k = 0, 1, \ldots, n/2, \text{ and} \\ \mathbf{x}[n-k] &= b_k, && \text{for } k = 1, 2, \ldots, n/2 - 1. \end{aligned}$$

If $n$ is odd then the sequence has one purely real element and, letting $n = 2s+1$, is stored as follows:

| Index of **x** | 0 | 1 | 2 | ... | $s$ | $s+1$ | ... | $n-2$ | $n-1$ |
|---|---|---|---|---|---|---|---|---|---|
| Sequence | $a_0$ | $a_1 + ib_1$ | $a_2 + ib_2$ | ... | $a_s + ib_s$ | $a_s - ib_s$ | ... | $a_2 - ib_2$ | $a_1 - ib_1$ |
| Stored values | $a_0$ | $a_1$ | $a_2$ | ... | $a_s$ | $b_s$ | ... | $b_2$ | $b_1$ |

$$\begin{aligned} \mathbf{x}[k] &= a_k, && \text{for } k = 0, 1, \ldots, s, \text{ and} \\ \mathbf{x}[n-k] &= b_k, && \text{for } k = 1, 2, \ldots, s. \end{aligned}$$

The second (recommended) storage scheme, referred to in this chapter as the **complex storage format** for Hermitian sequences, stores the real and imaginary parts $a_k, b_k$, for $0 \le k \le n/2$, in consecutive locations of an array **x** of length $n+2$. The following two tables illustrate the storage of the real and imaginary parts of $\hat{z}_k$ for the two cases: $n$ even and $n$ odd.

If $n$ is even then the sequence has two purely real elements and is stored as follows:

| Index of **x** | 0 | 1 | 2 | 3 | ... | $n-2$ | $n-1$ | $n$ | $n+1$ |
|---|---|---|---|---|---|---|---|---|---|
| Stored values | $a_0$ | $b_0 = 0$ | $a_1$ | $b_1$ | ... | $a_{n/2-1}$ | $b_{n/2-1}$ | $a_{n/2}$ | $b_{n/2} = 0$ |

$$\begin{aligned} \mathbf{x}[2 \times k - 1] &= a_k, && \text{for } k = 0, 1, \ldots, n/2, \text{ and} \\ \mathbf{x}[2 \times k + 1 - 1] &= b_k, && \text{for } k = 0, 1, \ldots, n/2. \end{aligned}$$

If $n$ is odd then the sequence has one purely real element and, letting $n = 2s+1$, is stored as follows:

| Index of **x** | 0 | 1 | 2 | 3 | ... | $n-2$ | $n-1$ | $n$ | $n+1$ |
|---|---|---|---|---|---|---|---|---|---|
| Stored values | $a_0$ | $b_0 = 0$ | $a_1$ | $b_1$ | ... | $b_{s-1}$ | $a_s$ | $b_s$ | 0 |

$$\begin{aligned}\mathbf{x}[2\times k-1] &= a_k, \quad \text{for } k=0,1,\ldots,s, \text{ and}\\ \mathbf{x}[2\times k+1-1] &= b_k, \quad \text{for } k=0,1,\ldots,s.\end{aligned}$$

Also, given a Hermitian sequence, the inverse (or backward) discrete transform produces a real sequence. That is,

$$x_j = \frac{1}{\sqrt{n}}\left(a_0 + 2\sum_{k=1}^{n/2-1}\left(a_k\cos\left(\frac{2\pi jk}{n}\right) - b_k\sin\left(\frac{2\pi jk}{n}\right)\right) + a_{n/2}\right)$$

where $a_{n/2} = 0$ if $n$ is odd.

For real data that is two-dimensional or higher, the symmetry in the transform persists for the leading dimension only. So, using the notation of equation (3) for the complex two-dimensional discrete transform, we have that $\hat{z}_{k_1k_2}$ is the complex conjugate of $\hat{z}_{(n_1-k_1)k_2}$. It is more convenient for transformed data of two or more dimensions to be stored as a complex sequence of length $(n_1/2+1)\times n_2\times\cdots\times n_d$ where $d$ is the number of dimensions. The inverse discrete Fourier transform operating on such a complex sequence (Hermitian in the leading dimension) returns a real array of full dimension $(n_1\times n_2\times\cdots\times n_d)$.

### 2.1.3 Real symmetric transforms

In many applications the sequence $x_j$ will not only be real, but may also possess additional symmetries which we may exploit to reduce further the computing time and storage requirements. For example, if the sequence $x_j$ is **odd**, $\left(x_j = -x_{n-j}\right)$, then the discrete Fourier transform of $x_j$ contains only sine terms. Rather than compute the transform of an odd sequence, we define the **sine transform** of a real sequence by

$$\hat{x}_k = \sqrt{\frac{2}{n}}\sum_{j=1}^{n-1} x_j\sin\left(\frac{\pi jk}{n}\right),$$

which could have been computed using the Fourier transform of a real odd sequence of length $2n$. In this case the $x_j$ are arbitrary, and the symmetry only becomes apparent when the sequence is extended. Similarly we define the **cosine transform** of a real sequence by

$$\hat{x}_k = \sqrt{\frac{2}{n}}\left(\tfrac{1}{2}x_0 + \sum_{j=1}^{n-1} x_j\cos\left(\frac{\pi jk}{n}\right) + \tfrac{1}{2}(-1)^k x_n\right)$$

which could have been computed using the Fourier transform of a real **even** sequence of length $2n$.

In addition to these 'half-wave' symmetries described above, sequences arise in practice with 'quarter-wave' symmetries. We define the **quarter-wave sine transform** by

$$\hat{x}_k = \frac{1}{\sqrt{n}}\left(\sum_{j=1}^{n-1} x_j\sin\left(\frac{\pi j(2k-1)}{2n}\right) + \tfrac{1}{2}(-1)^{k-1}x_n\right)$$

which could have been computed using the Fourier transform of a real sequence of length $4n$ of the form

$$(0, x_1, \ldots, x_n, x_{n-1}, \ldots, x_1, 0, -x_1, \ldots, -x_n, -x_{n-1}, \ldots, -x_1).$$

Similarly we may define the **quarter-wave cosine transform** by

$$\hat{x}_k = \frac{1}{\sqrt{n}}\left(\tfrac{1}{2}x_0 + \sum_{j=1}^{n-1} x_j\cos\left(\frac{\pi j(2k-1)}{2n}\right)\right)$$

which could have been computed using the Fourier transform of a real sequence of length $4n$ of the form

$$(x_0, x_1, \ldots, x_{n-1}, 0, -x_{n-1}, \ldots, -x_0, -x_1, \ldots, -x_{n-1}, 0, x_{n-1}, \ldots, x_1).$$

### 2.1.4 Fourier integral transforms

The usual application of the discrete Fourier transform is that of obtaining an approximation of the **Fourier integral transform**

$$F(s) = \int_{-\infty}^{\infty} f(t) \exp(-i2\pi st)\, dt$$

when $f(t)$ is negligible outside some region $(0, c)$. Dividing the region into $n$ equal intervals we have

$$F(s) \cong \frac{c}{n} \sum_{j=0}^{n-1} f_j \exp\left(\frac{-i2\pi sjc}{n}\right)$$

and so

$$F_k \cong \frac{c}{n} \sum_{j=0}^{n-1} f_j \exp\left(\frac{-i2\pi jk}{n}\right)$$

for $k = 0, 1, \ldots, n-1$, where $f_j = f(jc/n)$ and $F_k = F(k/c)$.

Hence the discrete Fourier transform gives an approximation to the Fourier integral transform in the region $s = 0$ to $s = n/c$.

If the function $f(t)$ is defined over some more general interval $(a, b)$, then the integral transform can still be approximated by the discrete transform provided a shift is applied to move the point $a$ to the origin.

### 2.1.5 Convolutions and correlations

One of the most important applications of the discrete Fourier transform is to the computation of the discrete **convolution** or **correlation** of two vectors $x$ and $y$ defined (as in Brigham (1974)) by

$$\text{convolution: } z_k = \sum_{j=0}^{n-1} x_j y_{k-j}$$

$$\text{correlation: } w_k = \sum_{j=0}^{n-1} \bar{x}_j y_{k+j}$$

(Here $x$ and $y$ are assumed to be periodic with period $n$.)

Under certain circumstances (see Brigham (1974)) these can be used as approximations to the convolution or correlation integrals defined by

$$z(s) = \int_{-\infty}^{\infty} x(t) y(s-t)\, dt$$

and

$$w(s) = \int_{-\infty}^{\infty} \bar{x}(t) y(s+t)\, dt, \quad -\infty < s < \infty.$$

For more general advice on the use of Fourier transforms, see Hamming (1962); more detailed information on the fast Fourier transform algorithm can be found in Gentleman and Sande (1966) and Brigham (1974).

### 2.1.6 Applications to solving partial differential equations (PDEs)

A further application of the fast Fourier transform, and in particular of the Fourier transforms of symmetric sequences, is in the solution of elliptic PDEs. If an equation is discretized using finite differences, then it is possible to reduce the problem of solving the resulting large system of linear equations to that of solving a number of tridiagonal systems of linear equations. This is accomplished by uncoupling the equations using Fourier transforms, where the nature of the boundary conditions determines the choice of transforms – see Section 3.3. Full details of the Fourier method for the solution of PDEs may be found in Swarztrauber (1977) and Swarztrauber (1984).

### 2.2 Direct Summation of Orthogonal Series

For any series of functions $\phi_i$ which satisfy a recurrence

$$\phi_{r+1}(x) + \alpha_r(x)\phi_r(x) + \beta_r(x)\phi_{r-1}(x) = 0$$

the sum

$$\sum_{r=0}^{n} a_r\phi_r(x)$$

is given by

$$\sum_{r=0}^{n} a_r\phi_r(x) = b_0(x)\phi_0(x) + b_1(x)(\phi_1(x) + \alpha_0(x)\phi_0(x))$$

where

$$b_r(x) + \alpha_r(x)b_{r+1}(x) + \beta_{r+1}(x)b_{r+2}(x) = a_r b_{n+1}(x) = b_{n+2}(x) = 0.$$

This may be used to compute the sum of the series. For further reading, see Hamming (1962).

## 3 Recommendations on Choice and Use of Available Functions

The fast Fourier transform algorithm ceases to be 'fast' if applied to values of $n$ which cannot be expressed as a product of small prime factors. All the FFT functions in this chapter are particularly efficient if the only prime factors of $n$ are 2, 3 or 5.

### 3.1 One-dimensional Fourier Transforms

The choice of function is determined first of all by whether the data values constitute a real, Hermitian or general complex sequence. It is wasteful of time and storage to use an inappropriate function.

#### 3.1.1 Real and Hermitian data

nag_sum_fft_realherm_1d (c06pac) transforms a single sequence of real data onto (and in-place) a representation of the transformed Hermitian sequence using the **complex storage scheme** described in Section 2.1.2. nag_sum_fft_realherm_1d (c06pac) also performs the inverse transform using the representation of Hermitian data and transforming back to a real data sequence.

Alternatively, the two-dimensional function nag_sum_fft_real_2d (c06pvc) can be used (on setting the second dimension to 1) to transform a sequence of real data onto an Hermitian sequence whose first half is stored in a separate Complex array. The second half need not be stored since these are the complex conjugate of the first half in reverse order. nag_sum_fft_hermitian_2d (c06pwc) performs the inverse operation, transforming the the Hermitian sequence (half-)stored in a Complex array onto a separate real array.

#### 3.1.2 Complex data

nag_sum_fft_complex_1d (c06pcc) transforms a single complex sequence in-place; it also performs the inverse transform. nag_sum_fft_complex_1d_multi (c06psc) transforms multiple complex sequences, each stored sequentially; it also performs the inverse transform on multiple complex sequences. This function is designed to perform several transforms in a single call, all with the same value of $n$.

If extensive use is to be made of these functions and you are concerned about efficiency, you are advised to conduct your own timing tests.

### 3.2 Half- and Quarter-wave Transforms

Four functions are provided for computing fast Fourier transforms (FFTs) of real symmetric sequences. nag_sum_fft_sine (c06rec) computes multiple Fourier sine transforms, nag_sum_fft_cosine (c06rfc) computes multiple Fourier cosine transforms, nag_sum_fft_qtrsine (c06rgc) computes multiple quarter-

wave Fourier sine transforms, and nag_sum_fft_qtrcosine (c06rhc) computes multiple quarter-wave Fourier cosine transforms.

## 3.3 Application to Elliptic Partial Differential Equations

As described in Section 2.1.6, Fourier transforms may be used in the solution of elliptic PDEs.

nag_sum_fft_sine (c06rec) may be used to solve equations where the solution is specified along the boundary.

nag_sum_fft_cosine (c06rfc) may be used to solve equations where the derivative of the solution is specified along the boundary.

nag_sum_fft_qtrsine (c06rgc) may be used to solve equations where the solution is specified on the lower boundary, and the derivative of the solution is specified on the upper boundary.

nag_sum_fft_qtrcosine (c06rhc) may be used to solve equations where the derivative of the solution is specified on the lower boundary, and the solution is specified on the upper boundary.

For equations with periodic boundary conditions the full-range Fourier transforms computed by nag_sum_fft_realherm_1d (c06pac) are appropriate.

## 3.4 Multidimensional Fourier Transforms

The following functions compute multidimensional discrete Fourier transforms of real, Hermitian and complex data stored in Complex arrays:

| | **double** | **Hermitian** | **Complex** |
|---|---|---|---|
| 2 dimensions | c06pvc | c06pwc | c06puc |
| 3 dimensions | c06pyc | c06pzc | c06pxc |
| any number of dimensions | | | c06pjc |

The Hermitian data, either transformed from or being transformed to real data, is compacted (due to symmetry) along its first dimension when stored in Complex arrays; thus approximately half the full Hermitian data is stored.

nag_sum_fft_complex_2d (c06puc) and nag_fft_3d (c06pxc) should be used in preference to nag_fft_multid_full (c06pjc) for two- and three-dimensional transforms, as they are easier to use and are likely to be more efficient.

The transform of multidimensional real data is stored as a complex sequence that is Hermitian in its leading dimension. The inverse transform takes such a complex sequence and computes the real transformed sequence. Consequently, separate functions are provided for performing forward and inverse transforms.

nag_sum_fft_real_2d (c06pvc) performs the forward two-dimensionsal transform while nag_sum_fft_hermitian_2d (c06pwc) performs the inverse of this transform.

nag_sum_fft_real_3d (c06pyc) performs the forward three-dimensional transform while nag_sum_fft_hermitian_3d (c06pzc) performs the inverse of this transform.

The complex sequences computed by nag_sum_fft_real_2d (c06pvc) and nag_sum_fft_real_3d (c06pyc) contain roughly half of the Fourier coefficients; the remainder can be reconstructed by conjugation of those computed. For example, the Fourier coefficients of the two-dimensional transform $\hat{z}_{(n_1-k_1)k_2}$ are the complex conjugate of $\hat{z}_{k_1k_2}$ for $k_1 = 0, 1, \ldots, n_1/2$, and $k_2 = 0, 1, \ldots, n_2 - 1$.

## 3.5 Convolution and Correlation

nag_sum_convcorr_real (c06fkc) computes either the discrete convolution or the discrete correlation of two real vectors.

### 3.6 Direct Summation of Orthogonal Series

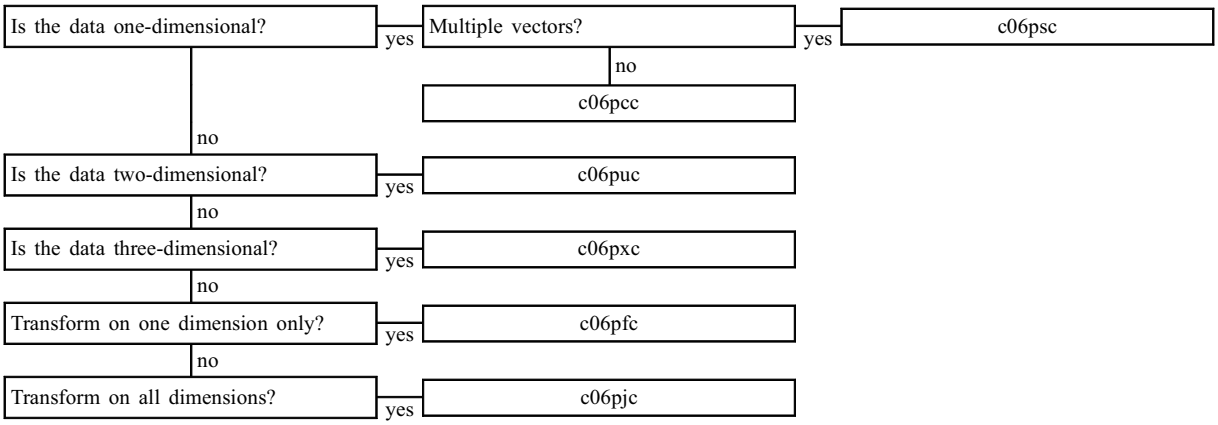
The only function available is nag_sum_cheby_series (c06dcc), which sums a finite Chebyshev series

$$\sum_{j=0}^{n} c_j T_j(x), \quad \sum_{j=0}^{n} c_j T_{2j}(x) \quad \text{or} \quad \sum_{j=0}^{n} c_j T_{2j+1}(x)$$

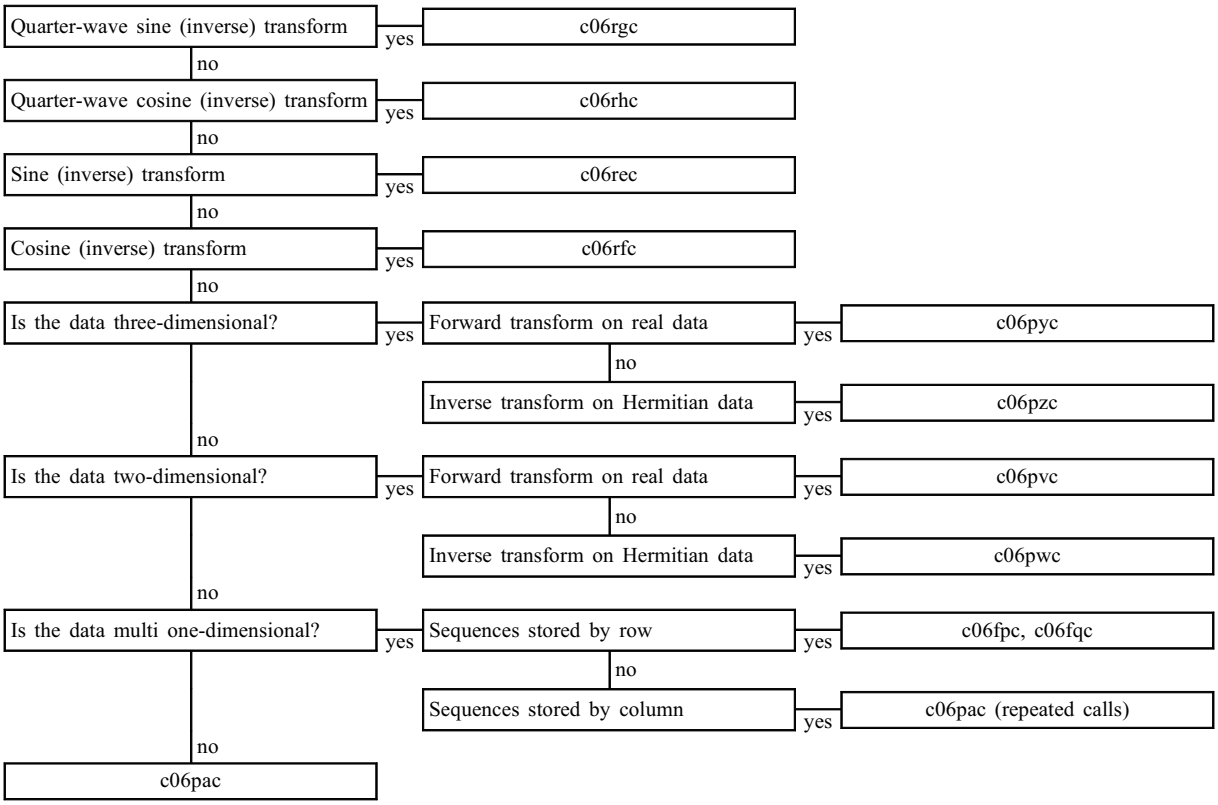
depending on the choice of an argument.

## 4 Decision Trees

**Tree 1: Fourier Transform of Discrete Complex Data**




**Tree 2: Fourier Transform of Real Data or Data in Complex Hermitian Form Resulting from the Transform of Real Data**



## 5 Functionality Index



## 6 Auxiliary Functions Associated with Library Function Arguments

None.

# 7 Functions Withdrawn or Scheduled for Withdrawal

The following lists all those functions that have been withdrawn since Mark 23 of the Library or are scheduled for withdrawal at one of the next two marks.

| Withdrawn Function | Mark of Withdrawal | Replacement Function(s) |
|---|---|---|
| nag_fft_real (c06eac) | 26 | nag_sum_fft_realherm_1d (c06pac) |
| nag_fft_hermitian (c06ebc) | 26 | nag_sum_fft_realherm_1d (c06pac) |
| nag_fft_complex (c06ecc) | 26 | nag_sum_fft_complex_1d (c06pcc) |
| nag_convolution_real (c06ekc) | 26 | nag_sum_convcorr_real (c06fkc) |
| nag_fft_multiple_complex (c06frc) | 26 | nag_sum_fft_complex_1d_multi (c06psc) |
| nag_fft_2d_complex (c06fuc) | 26 | nag_sum_fft_complex_2d (c06puc) |
| nag_conjugate_hermitian (c06gbc) | 26 | No replacement required |
| nag_conjugate_complex (c06gcc) | 26 | No replacement required |
| nag_fft_multiple_sine (c06hac) | 26 | nag_sum_fft_sine (c06rec) |
| nag_fft_multiple_cosine (c06hbc) | 26 | nag_sum_fft_cosine (c06rfc) |
| nag_fft_multiple_qtr_sine (c06hcc) | 26 | nag_sum_fft_qtrsine (c06rgc) |
| nag_fft_multiple_qtr_cosine (c06hdc) | 26 | nag_sum_fft_qtrcosine (c06rhc) |

# 8 References

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