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Evaluation of incomplete gamma functions using downward recursion and analytical relations

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New downward recursion and analytical approaches are presented for the calculation of incomplete gamma functions $\gamma(\alpha, x)$ and $\Gamma(\alpha, x)$. The efficiency of calculation with an adequate interval of these expressions is compared with those of other methods and great numerical stability and good rate of convergence is obtained for wide range of integral parameters. It is shown that the downward recursive relations are stable for all values of α and x of $\gamma(\alpha, x)$.

KEY WORDS: incomplete gamma functions, downward recursion relations, molecular auxiliary functions, overlap integrals, noninteger principal quantum numbers

AMS subject classification: 81-08, 81-V55, 81V45

1. Introduction

It is well known that the computation of incomplete gamma functions (IGFs) is a significant component of the overall cost of many ab initio algorithm [1–7] and applied science [8–25]. These functions have already been investigated by numerous authors with different algorithms [26–41]. Although, the methods used by these authors have a simple form, inefficiency arises in the evaluation of incomplete gamma function $\gamma(\alpha, x)$ especially for $(\alpha/x) > 1$. The purpose of this paper is to present an accurate algorithm for the evaluation of IGFs with arbitrary values of parameters α and x using downward recursion relations and analytical formulas.

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2. Definitions and downward recursion approach

The incomplete gamma functions examined in the present work are defined by [42]:

$$\gamma(\alpha, x) = \int_0^x t^{\alpha-1} \mathrm{e}^{-t}\, \mathrm{d}t, \tag{1}$$

$$\Gamma(\alpha, x) = \int_x^\infty t^{\alpha-1} \mathrm{e}^{-t}\, \mathrm{d}t, \tag{2}$$

where $x > 0, \alpha = n + \varepsilon, 0 \leqslant \varepsilon < 1$ and $n = 1, 2, \ldots$ These functions are related to each other by

$$\gamma(\alpha, x) + \Gamma(\alpha, x) = \Gamma(\alpha), \tag{3}$$

where $\Gamma(\alpha)$ is the gamma function determined as

$$\Gamma(\alpha) = \int_0^\infty t^{\alpha-1} \mathrm{e}^{-t}\, \mathrm{d}t. \tag{4}$$

The incomplete gamma functions $\gamma(\alpha, x)$ and $\Gamma(\alpha, x)$ satisfy the following recursive relations:
Upward recurrences

$$\gamma(\alpha, x) = (\alpha - 1)\gamma(\alpha - 1, x) - \mathrm{e}^{-x} x^{\alpha-1}, \tag{5}$$

$$\Gamma(\alpha, x) = (\alpha - 1)\Gamma(\alpha - 1, x) - \mathrm{e}^{-x} x^{\alpha-1}, \tag{6}$$

$$C(\alpha, x) = \alpha C(\alpha - 1, x) + x^{\alpha}, \tag{7}$$

where

$$\Gamma(\alpha, x) = \mathrm{e}^{-x} C(\alpha - 1, x). \tag{8}$$

Downward recurrences

$$\gamma(\alpha, x) = [\gamma(\alpha + 1, x) - \mathrm{e}^{-x} x^{\alpha}]/\alpha, \tag{9}$$

$$\Gamma(\alpha, x) = [\Gamma(\alpha + 1, x) - \mathrm{e}^{-x} x^{\alpha}]/\alpha, \tag{10}$$

$$C(\alpha, x) = [C(\alpha + 1, x) - x^{\alpha+1}]/(\alpha + 1). \tag{11}$$

The starting terms in equations (5)–(7) are given by

$$\gamma(1 + \varepsilon, x) = \begin{cases} 1 - \mathrm{e}^{-x} & \text{for } \varepsilon = 0 \\ \sum\limits_{m=0}^{\infty} \frac{(-1)^m x^{1+\varepsilon+m}}{m!(1+\varepsilon+m)} & \text{for } 0 < \varepsilon < 1 \end{cases} \tag{12}$$

$$\Gamma(1 + \varepsilon, x) = \begin{cases} \mathrm{e}^{-x} & \text{for } \varepsilon = 0, \quad (13) \\ \Gamma(1 + \varepsilon) - \gamma(1 + \varepsilon, x) & \text{for } 0 < \varepsilon < 1, \quad (14) \end{cases}$$

$$C(\varepsilon, x) = \mathrm{e}^x \Gamma(1+\varepsilon, x). \tag{15}$$

In this work, the incomplete gamma functions $\gamma(\alpha, x)$ and $\Gamma(\alpha, x)$ are evaluated and analyzed in range of $0 < \alpha \leqslant 100$ and $0.001 \leqslant x \leqslant 100$. For $x \geqslant 0.01$ and $x \leqslant 0.01$ values, the function $\Gamma(\alpha, x)$ is calculated from the upward recursive relations (6) and (7), respectively. The recurrence relation (5) for $\gamma(\alpha, x)$ becomes unstable when $(n/x) > 1$. The absolute error made in the initial value $\gamma(1+\varepsilon, x)$ in equation (5) grows with a factor n/x in each step. This difficulty can be overcome by using the recursive relation downward for $(n/x) > 1$. The computer calculations for $(n/x) > 1$ show that the downward relation (9) gives more accurate results. By the use of method set out in Ref. [43] it is easy to show that as a result of having d significant digits in $\gamma(n_{\max} + \varepsilon, x)$ the downward recursion should be started from the even value of n_t satisfying

$$n_t \geqslant \begin{cases} \frac{d}{|\log(n_{\max}/x)|} + n_{\max} & \text{for } n_{\max} \neq x, & (16)\\ \frac{d}{|\log(n_{\max})|} + n_{\max} & \text{for } n_{\max} = x, & (17)\end{cases}$$

$$\gamma(n_t + \varepsilon, x) \cong \gamma(1+\varepsilon, x). \tag{18}$$

3. Analytical approach

Now we move on to the determination of analytical relations for the functions $\gamma(\alpha, x)$ and $\Gamma(\alpha, x)$ in terms of their initial values determined by equations (12)–(15). For this purpose we use the recursive formulas (5) and (6) in the following form:

$$\gamma(\alpha, x) = (\alpha)_k \gamma(\alpha - k, x) - \mathrm{e}^{-x} \sum_{i=1}^{k} (\alpha)_{k-i} x^{\alpha-k+i-1}, \tag{19}$$

$$\Gamma(\alpha, x) = (\alpha)_k \Gamma(\alpha - k, x) + \mathrm{e}^{-x} \sum_{i=1}^{k} (\alpha)_{k-i} x^{\alpha-k+i-1}, \tag{20}$$

where

$$(\alpha)_k = \begin{cases} 1 & \text{for } k = 0, & (21)\\ (\alpha-1)(\alpha-2)\cdots(\alpha-k) & \text{for } 1 \leqslant k \leqslant n-1. & (22)\end{cases}$$

By considering the particular case of equations (19) and (20) with $k = n-1$ we finally obtain for the incomplete gamma functions the relationships in terms of initial values:

$$\gamma(n+\varepsilon, x) = (n+\varepsilon)_{n-1}\gamma(1+\varepsilon, x) - \mathrm{e}^{-x}\sum_{i=1}^{n-1}(n+\varepsilon)_{n-1-i}x^{\varepsilon+i}, \tag{23}$$

$$\Gamma(n+\varepsilon, x) = (n+\varepsilon)_{n-1}\Gamma(1+\varepsilon, x) + \mathrm{e}^{-x}\sum_{i=1}^{n-1}(n+\varepsilon)_{n-1-i}x^{\varepsilon+i}. \tag{24}$$

Taking into account equations (19), (20), (23), and (24) in equation (3) it is easy to establish for the complete gamma functions the following relations:

$$\Gamma(\alpha) = (\alpha)_k\Gamma(\alpha-k), \tag{25}$$

$$\Gamma(n+\varepsilon) = (n+\varepsilon)_{n-1}\Gamma(1+\varepsilon), \tag{26}$$

where [23,42]

$$\Gamma(1+\varepsilon) = \begin{cases} 1 & \text{for } \varepsilon = 0, \\ \varepsilon\,\Gamma(\varepsilon) & \text{for } 0 < \varepsilon < 1. \end{cases} \tag{27}$$

4. Numerical calculations and discussion

New approaches have been presented for the computation of incomplete gamma functions that arise in theoretical and applied science. These approaches can be used for arbitrary integer and noninteger values of indices α and x.

On the basis of formulas obtained in this paper we constructed a program for computation of incomplete gamma functions $\gamma(\alpha, x)$ and $\Gamma(\alpha, x)$ on a Pentium III 800 MHz (using Turbo Pascal language). One can determine the accuracy of the computer results obtained from the upward recurrences (downward recurrences) by the use of the downward recurrences (upward recurrences). The examples of computer calculation for the $\gamma(\alpha, x)$ are shown in Table 1. The numbers of correct decimal figures m_u and m_d determined from $\Delta f_u = 10^{-m_u}$ and $\Delta f_d = 10^{-m_d}$ are given in this table, where $\Delta f = f^{\mathrm{L}} - f^{\mathrm{R}}$. Here, the values f^{L} and f^{R} are obtained from the left-hand side (LHS) and the right-hand side (RHS) of above mentioned equations, respectively.

As can be seen from the table, our results are in excellent agreement with the results Maple 7 and Mathematica 4 international mathematical software. Hopefully, this simplification will persist at higher orders. We have tested the program by comparing with much available data Maple 7 and Mathematica 4 international mathematical software.

Table 1
Numbers of correct decimal figures for incomplete gamma functions $\gamma(\alpha, x)$.

α	x	Equation (9)	Equation (23)	Maple 7.0	Mathematica 4
4	9	∞	∞	∞	∞
12	0.09	32		32	31
15	20	∞	∞	∞	∞
17	35	∞	∞	∞	∞
28	65	∞	∞	∞	∞
45	54.4	∞	∞	∞	∞
8	4.6	∞	∞	∞	∞
80	0.6	38		27	38
20	0.003	68		∞	48
7.25	10.5	∞	∞	∞	∞
12.5	5.55	∞	∞	∞	∞
20.2	0.17	31		34	34
64.2	53.3	∞	∞	∞	∞
25.7	25.7	∞	∞	∞	∞
25.8	30.5	∞	∞	∞	∞
1.8	25.5	∞	∞	∞	∞
3.2	100.3	∞	∞	∞	∞
95.7	100.3	∞	∞	∞	∞
8.6	45.5	∞	∞	∞	∞
0.001	25.7	∞		∞	∞

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