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Numerical quadrature for integrals involving oscillating functions

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Abstract

This paper deals with the construction of a coupled Gaussian rule for weight functions involving powers, exponentials and trigonometric functions. Starting from a recursive relation for the moments, nodes and weights are computed by using the Chebyshev algorithm together with the Golub and Welsch method. An a posteriori approximation of the quadrature error by means of the generalized averaged Gaussian rules is also considered. Several numerical examples are provided.

Keywords: Gaussian quadrature, Fourier type integral, averaged Gaussian rule (MSC2020: 65D32, 33C45)

1 Introduction

This work deals with the computation of

$$J(g) = \int_0^{+\infty} g(x) x^{\alpha - 1} e^{-\beta x} \cos\left(\omega x\right) dx, \quad \alpha > 0, \ \beta > 0, \ \omega > 0,$$
(1)

where g is a smooth function. The above integral can be also interpreted as the cosine transform (see [16]) of the function $g(x)x^{\alpha-1}e^{-\beta x}$ and it is typically referred to as a Fourier type integral, with a broad range of applications in signal processing. More specifically, integrals of type (1) arise for instance in geophysical electromagnetic survey (see e.g. [15]). In particular, the electromagnetic fields induced by an infinite line of electric current placed above the earth surface can be expressed as in (1), in which the function g encodes the reflection and refraction of the electromagnetic waves and depends on the properties of the subsoil structure. Such kind of source is used to simulate a long grounded wire or one side of a large rectangular loop.

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By using the simple change of variable $\omega x = t$, we reformulate the problem in the evaluation of integrals of type

$$I(f) = \int_0^{+\infty} f(t)t^{\alpha - 1}e^{-ct}\cos t \, dt = \omega^{\alpha}J(g),\tag{2}$$

with $c = \frac{\beta}{\omega}$, $f(t) = g(\frac{t}{\omega})$. In this way the frequency is inherited by the scale factor c. Working with formulation (2), in this paper we construct a coupled Gaussian rule, by first considering the positive weight function

$$w(t) = t^{\alpha - 1} e^{-ct} \left(\cos t + 1 \right), \tag{3}$$

and, then, by rewriting integral (2) as

$$I(f) = I^C(f) - I^L(f),$$

with

$$I^{C}(f) = \int_{0}^{+\infty} f(t)t^{\alpha - 1}e^{-ct}\left(\cos t + 1\right)dt,$$
(4)

and

$$I^{L}(f) = \int_{0}^{+\infty} f(t)t^{\alpha - 1}e^{-ct}dt = \frac{1}{c^{\alpha}}\int_{0}^{+\infty} f\left(\frac{y}{c}\right)y^{\alpha - 1}e^{-y}dy.$$
 (5)

We notice that the integral $I^{L}(f)$ can be accurately computed by using the generalized Gauss-Laguerre formula, that we denote by $I_{n}^{L}(f)$. Therefore, we focus on the construction of a Gaussian quadrature rule with respect to the weight function (3). Having at disposal such a formula, denoted by $I_{n}^{C}(f)$, we then consider the approximation

$$I(f) = \left(I_n^C(f) - I_n^L(f)\right) + E_n(f),\tag{6}$$

where $E_n(f)$ is the quadrature error.

In this setting, since we do not have at disposal the explicit expression of the orthogonal polynomials π_k , $k \ge 0$, relative to w(t) as in (3), we need to employ a numerical scheme to compute the coefficients of the three-term recursion

$$\begin{aligned} \pi_{k+1}(t) &= (t - \alpha_k) \pi_k(t) - \beta_k \pi_{k-1}(t), \quad k \ge 0, \\ \pi_{-1}(t) &= 0, \quad \pi_0(t) = 1, \end{aligned}$$

with $\beta_k > 0$. This can be done by evaluating the associated moments

$$\mu_k = \int_0^{+\infty} t^k w(t) dt, \quad k \ge 0, \tag{7}$$

and then by using the Chebyshev algorithm [4, sect. 2.3]. The coefficients α_k , β_k , $k \ge 0$, define the tridiagonal symmetric Jacobi matrix, whose eigenvalue decomposition provides abscissas and weights of the quadrature rule. This final step is efficiently implemented by the famous Golub and Welsch algorithm [7].

In order to approximate the quadrature error, we consider the corresponding generalized averaged Gaussian rules (see [14, 12, 13, 3]). These formulas provide an a posteriori estimate of the error. Moreover, they are easy to construct and typically lead to quite accurate approximations (see [12]).

We point out that all the results presented in the paper can be easily extended to the case of integrals as in (1), with the cosine replaced by the sine function (see also Remark 2).

The Matlab codes for the computation of integrals of type (2) by using the approximation (6) are available at https://github.com/EleonoraDe/Fourier-type-integrals.

The paper is organized as follows. In Section 2 we derive a recursive relation for the evaluation of the moments and show how to construct the coupled Gaussian formula. Some numerical experiments, in which we compare the rule with other methods, are provided in Section 3. In Section 4 we employ the generalized averaged Gaussian formulas to obtain an a posteriori estimate of the quadrature error. Concluding remarks can be found in Section 5.

2 Construction of the Gaussian formula

In order to develop the Gaussian quadrature rule, relative to the weight function (3), first of all we need to compute the moments

$$\mu_k = \int_0^{+\infty} t^{\alpha+k-1} e^{-ct} \left(\cos t + 1\right) dt, \quad k \ge 0.$$
(8)

Proposition 1. The following recursion holds

$$\mu_{0} = \frac{\Gamma(\alpha)}{c^{\alpha}} \left(\cos(\alpha \varphi) (\cos \varphi)^{\alpha} + 1 \right),$$

$$\mu_{k} = \frac{k - 1 + \alpha}{c} \frac{\cos((k + \alpha)\varphi) (\cos \varphi)^{k + \alpha} + 1}{\cos((k - 1 + \alpha)\varphi) (\cos \varphi)^{k - 1 + \alpha} + 1} \mu_{k - 1}, \quad k \ge 1,$$
(9)

with $\varphi = \arctan \frac{1}{c}$ and where Γ is the Gamma function.

Proof. First of all, from [8, p.490, 3.944, n.6], for the so called core moments (see [6, sect. 2.1]), defined by

$$\mu_{k,0} = \int_0^{+\infty} t^{\alpha+k-1} e^{-ct} \cos t \, dt, \quad k \ge 0, \tag{10}$$

we have that

$$\mu_{k,0} = \frac{\Gamma(k+\alpha)}{(1+c^2)^{\frac{k+\alpha}{2}}}\cos((k+\alpha)\varphi), \quad k \ge 0, \ \varphi = \arctan\frac{1}{c}.$$

Then, by definitions (8)-(10) and by using [8, sect. 3.381, n.4], for the moments μ_k , $k \ge 0$, we have

$$\mu_{k} = \mu_{k,0} + \int_{0}^{+\infty} t^{\alpha+k-1} e^{-ct} dt$$

= $\Gamma(k+\alpha) \left(\frac{\cos((k+\alpha)\varphi)}{(1+c^{2})^{\frac{k+\alpha}{2}}} + \frac{1}{c^{k+\alpha}} \right)$
= $\Gamma(k+\alpha) \frac{\cos((k+\alpha)\varphi)c^{k+\alpha} + (1+c^{2})^{\frac{k+\alpha}{2}}}{(c(1+c^{2}))^{\frac{k+\alpha}{2}}}$ (11)

Defining, for simplicity of notation,

$$d_k := \frac{\cos((k+\alpha)\varphi)c^{k+\alpha} + (1+c^2)^{\frac{k+\alpha}{2}}}{(c(1+c^2))^{\frac{k+\alpha}{2}}}, \quad k \ge 0,$$



Figure 1: Comparison between formula (9) (dashed line) and formula (11) (solid line) for the computation of the first 80 moments, with $\alpha = 0.7$ and c = 0.1. The plots show the relative errors with respect to a reference value computed by employing formula (9) with extended precision arithmetic (50 digits).

so that $\mu_k = \Gamma(k + \alpha)d_k$, after some computations, we have that

$$\frac{d_k}{d_{k-1}} = \frac{1}{c} \frac{\cos((k+\alpha)\varphi)(\cos\varphi)^{k+\alpha}+1}{\cos((k-1+\alpha)\varphi)(\cos\varphi)^{k-1+\alpha}+1}.$$

By using the above relation and formula (11), we obtain the result.

We notice that (11) gives an explicit expression for the computation of the moments μ_k , $k \ge 0$. Anyway, this formula involves the evaluation of the Gamma function and, from our numerical experiments, for growing k it seems a little less stable than the recursive relation (9) (see Figure 1).

Remark 2. A similar result can be derived also in the case the cosine in (2) is replaced by the sine function. In this situation, for the moments

$$\tilde{\mu}_k = \int_0^{+\infty} t^{\alpha+k-1} e^{-ct} \left(\sin t + 1\right) dt, \quad k \ge 0,$$

it holds

$$\begin{split} \tilde{\mu}_0 &= \frac{\Gamma(\alpha)}{c^{\alpha}} \left(\sin(\alpha \varphi) (\cos \varphi)^{\alpha} + 1 \right), \\ \tilde{\mu}_k &= \frac{k - 1 + \alpha}{c} \frac{\sin((k + \alpha)\varphi) (\cos \varphi)^{k + \alpha} + 1}{\sin((k - 1 + \alpha)\varphi) (\cos \varphi)^{k - 1 + \alpha} + 1} \mu_{k-1}, \quad k \ge 1, \end{split}$$

with $\varphi = \arctan \frac{1}{c}$ (see [8, p.490, 3.944, n.5]).

At this point, for the computation of the coefficients α_k and β_k of the recurrence relation

$$\pi_{k+1}(t) = (t - \alpha_k)\pi_k(t) - \beta_k\pi_{k-1}(t), \quad k \ge 0, \pi_{-1}(t) = 0, \quad \pi_0(t) = 1,$$

with $\beta_k > 0$, we employ the Chebyshev algorithm (see [4, sect. 2.3] and [5]). Given the first 2n moments $\mu_0, \ldots, \mu_{2n-1}$, this algorithm uniquely determines the first *n* recurrence coefficients α_k and β_k , $k = 0, \ldots, n-1$, by using the mixed moments defined as

$$\sigma_{kl} = \int_0^\infty \pi_k(t) t^l w(t) dt, \quad k, l \ge -1.$$

The Chebyshev algorithm is summarized in Algorithm 3. *Algorithm* 3. Initialization

$$egin{aligned} lpha_0 &= rac{\mu_1}{\mu_0}, \ eta_0 &= \mu_0, \ \sigma_{-1,l} &= 0, \quad l = 1, 2, \dots, 2n-2, \ \sigma_{0,l} &= \mu_l, \quad 0, 1, \dots, 2n-1, \end{aligned}$$

for k = 1, 2, ..., n - 1

for l = k, k + 1, ..., 2n - k - 1

$$egin{aligned} &\sigma_{k,l}=\sigma_{k-1,l+1}-lpha_{k-1}\sigma_{k-1,l}-eta_{k-1}\sigma_{k-2,l},\ &lpha_k=rac{\sigma_{k,k+1}}{\sigma_{k,k}}-rac{\sigma_{k-1,k}}{\sigma_{k-1,k-1}}, \quad η_k=rac{\sigma_{k,k}}{\sigma_{k-1,k-1}}. \end{aligned}$$

After the computation of α_k , β_k , k = 0, ..., n-1, the eigendecomposition of the corresponding Jacobi matrix

$$J_{n} = \begin{bmatrix} \alpha_{0} & \sqrt{\beta_{1}} & & 0\\ \sqrt{\beta_{1}} & \alpha_{1} & \sqrt{\beta_{2}} & & \\ & \sqrt{\beta_{2}} & \alpha_{2} & \ddots & \\ & & \ddots & \ddots & \sqrt{\beta_{n-1}}\\ 0 & & & \sqrt{\beta_{n-1}} & \alpha_{n-1} \end{bmatrix} \in \mathbb{R}^{n \times n},$$
(12)

provides the nodes $t_i^{(n)}$ and weights $w_i^{(n)}$, i = 1, ..., n, of the *n*-point Gaussian rule (see [1]). Then, for the computation of integral (4) we use the approximation

$$I^{C}(f) = I^{C}_{n}(f) + E^{C}_{n}(f) = \sum_{i=1}^{n} w^{(n)}_{i} f\left(t^{(n)}_{i}\right) + E^{C}_{n}(f).$$
(13)

As for integral (5), denoting by $\lambda_i^{(n)}$, $\xi_i^{(n)}$, i = 1, ..., n, the nodes and weights of the *n*-point generalized Gauss-Laguerre rule, we consider the approximation

$$I^{L}(f) = I^{L}_{n}(f) + E^{L}_{n}(f) = \frac{1}{c^{\alpha}} \sum_{i=1}^{n} \xi^{(n)}_{i} f\left(\frac{\lambda^{(n)}_{i}}{c}\right) + E^{L}_{n}(f).$$
(14)

In (13) and (14) $E_n^C(f)$ and $E_n^L(f)$ denote the corresponding quadrature errors. Finally, for integral (2) we obtain the rule (6), in which $E_n(f) = E_n^C(f) - E_n^L(f)$, that we call coupled Gaussian formula.

3 Numerical experiments

In this section we provide some numerical examples in which we test the performances of the developed coupled Gaussian rule. We start by observing that, by using the change of variable x = ct in (2), which leads to

$$I(f) = I_c(h) = \frac{1}{c^{\alpha}} \int_0^{+\infty} h(x) x^{\alpha - 1} e^{-x} dx, \quad h(x) = f\left(\frac{x}{c}\right) \cos\left(\frac{x}{c}\right),$$

and by considering as weight function

$$w^{GL}(x) = x^{\alpha - 1} e^{-x},$$

integral (2) can be evaluated by employing the *n*-point generalized Gauss-Laguerre formula, that is,

$$I_n^{GL}(h) = \frac{1}{c^{\alpha}} \sum_{i=1}^n h\left(\lambda_i^{(n)}\right) \xi_i^{(n)},$$
(15)

so that $I(f) = I_n^{GL}(f) + E_n^{GL}(h)$, where $E_n^{GL}(h)$ denotes the quadrature error. As for the computation of the nodes and weights of the generalized Gauss-Laguerre rule, we have used the Matlab routine lagpts.m of the Chebfun package (see. [2]) In this view, in Figures 2-3-4 we compare the behavior of the coupled Gaussian rule (6) with (15), with respect to a reference solution. In other words, as a first set of experiments we compare formula (6) with the Laguerre rule in which the oscillating term is not part of the weight function. Different sets of parameters and functions f are considered. All the computations are carried out in Matlab by using extended precision arithmetic. Indeed, it is known that the computation of the coefficients α_k , β_k is a severely ill-conditioned problem, even for k not too large (see e.g. [5]).

We remark that formula (6) requires a double set of points and therefore a double number of function evaluations. Nevertheless, by looking at the figures, we observe that this formula is typically more accurate than the generalized Gauss-Laguerre formula, especially for small values of the parameter c (see Figures 2a-3-4a). Recalling that $c = \frac{\beta}{\omega}$ in (2), this parameter handles the scale and, therefore, the frequency of oscillations (cf. (1)-(2)). For large c method (6) is less effective since the Laguerre rule appears to be reliable for slow oscillations (see Figures 2b-4b).

As already mentioned in the Introduction, integral (1) can be interpreted as the cosine transform

$$I(F, \boldsymbol{\omega}) = \int_0^{+\infty} F(x) \cos(\boldsymbol{\omega} x) dx,$$
(16)

with $F(x) = g(x)x^{\alpha-1}e^{-\beta x}$. An efficient method for the computation of (16) where the function *F* is slowly decaying is based on the use of the double exponential transformation (see [10, 9])

$$x = rac{M\Phi\left(t - rac{\pi}{2M}
ight)}{\omega}, \quad M > 0, \quad \Phi(\zeta) = rac{\zeta}{1 - e^{-2\pi \sinh \zeta}},$$

that leads to

$$I(F,\omega) = \frac{M}{\omega} \int_{-\infty}^{+\infty} F\left(\frac{M\Phi\left(t - \frac{\pi}{2M}\right)}{\omega}\right) \cos\left(M\Phi\left(t - \frac{\pi}{2M}\right)\right) \Phi'\left(t - \frac{\pi}{2M}\right) dt.$$



Figure 2: Comparison between the absolute error obtained by using the coupled Gaussian approach (6) and the Gauss-Laguerre formula (15) for $\alpha = 1.1$, c = 0.2 (left) and $\alpha = 0.5$, c = 0.4 (right). In both cases $f(t) = \frac{1}{1+e^{-t}}$.



Figure 3: Comparison between the absolute error obtained by using the coupled Gaussian approach (6) and the Gauss-Laguerre formula (15) for $\alpha = 1.5$, c = 0.05 (left) and $\alpha = 1.3$, c = 0.1 (right). In both cases $f(t) = \frac{1}{1+t}$.



Figure 4: Comparison between the absolute error obtained by using the coupled Gaussian approach (6) and the Gauss-Laguerre formula (15) for $\alpha = 0.5$, c = 0.2 (left) and $\alpha = 1.3$, c = 0.7 (right). In both cases $f(t) = e^{-0.5t^2}$.

The idea was then to consider the trapezoidal rule with step τ and suitable truncation. By setting $M\tau = \pi$ as in [11], the method reads

$$I_{N}(F) = \frac{\pi}{\omega} \sum_{n=-N}^{N} F\left(\frac{M\Phi\left(\left(n-\frac{1}{2}\right)\frac{\pi}{M}\right)}{\omega}\right) \cos\left(M\Phi\left(\left(n-\frac{1}{2}\right)\frac{\pi}{M}\right)\right) \times \Phi'\left(\left(n-\frac{1}{2}\right)\frac{\pi}{M}\right).$$
(17)

This rule can be very efficient but requires the proper selection of τ (*M*) and *N*. This corresponds to locate the significant support of the function with respect to the required accuracy and to define a suitable discretization. As for the sine transform

$$I(F,\omega) = \int_0^{+\infty} F(x) \sin(\omega x) dx,$$

the method is almost identical with the only difference in the initial substitution, that now reads

$$x = \frac{M\Phi(t)}{\omega}.$$

Assuming $\omega = 1$ and taking $F(x) = f(x)x^{\alpha-1}e^{-cx}$, we have $I(F, \omega) = I(f)$ (cf. (2)-(16)). In this setting, in Figures 5-6-7 we report some results, where we compare our coupled Gaussian method with the trapezoidal rule for different sets of parameters. In all pictures we consider the results of the trapezoidal rule for M = 4, 8, 12, ... in order to reduce the step, and then $N = \frac{M}{2}, M, \frac{3}{2}M$ to work with increasing number of points, that is, by reducing the truncation errors. As for the coupled Gaussian approach, we truncate rules (13)-(14) by neglecting the terms for which the values of the weights $w_i^{(n)}, \lambda_i^{(n)}, i = 1, ..., n$, are less than 1e - 16. Depending on the function f and on the parameters, the trapezoidal rule appears to be extremely sensitive with respect to the choice of N. For small N it shows a very fast initial convergence but also stagnation, while for larger N the attainable accuracy is higher, but the method is slower (see Figure 5). Basically, the Gaussian approach appears preferable for α , c and f such that the



Figure 5: Comparison between the absolute error obtained by using the coupled Gaussian rule (6) and the trapezoidal rule based on the double exponential transform (17) for $\alpha = 1.3$, c = 0.7 (left) and $\alpha = 1.3$, c = 0.3 (right). In both cases $f(t) = e^{-0.5t^2}$.

support is relatively large (Figures 5-6a), whereas the trapezoidal rule is more effective for functions rapidly decaying (Figure 6b and other experiments non reported). Figure 7 shows a situation in which both methods are not much accurate because of the high frequency of oscillations.

4 A posteriori error estimate

In this section, we construct the generalized averaged Gaussian rules A_{2n+1}^C , A_{2n+1}^L (see [14]), associated with the Gaussian formulas I_n^C , I_n^L , respectively, and employ them to approximate the quadrature error

$$E_n(f) = I(f) - \left(I_n^C(f) - I_n^L(f)\right).$$
 (18)

The generalized averaged Gaussian formula A_{2n+1} , associated with a generic Gaussian rule I_n is given by (see [12])

$$A_{2n+1}(f) = \frac{b_{n+1}}{b_n + b_{n+1}} I_n(f) + \frac{b_n}{b_n + b_{n+1}} \tilde{A}_{n+1}(f),$$

where the quadrature formula

$$\tilde{A}_{n+1}(f) = \sum_{i=1}^{n+1} \sigma_i^{(n+1)} f\left(\tau_i^{(n+1)}\right)$$
(19)

arises from the symmetric tridiagonal matrix $ilde{J}_{n+1} \in \mathbb{R}^{(n+1) imes (n+1)}$, defined as

$$\tilde{J}_{n+1} = \begin{bmatrix} J_n & e_n \sqrt{b_n + b_{n+1}} \\ e_n^T \sqrt{b_n + b_{n+1}} & a_n \end{bmatrix},$$
(20)

in which $e_n = (0, ..., 0, 1)^T \in \mathbb{R}^n$, J_n is as in (12) and $a_k, b_k, k \ge 0$, are the coefficients of the corresponding three-term recurrence relation of the orthogonal system $\{p_k\}_{k>0}$ associated with



Figure 6: Comparison between the absolute error obtained by using the coupled Gaussian rule (6) and the trapezoidal rule based on the double exponential transform (17) for $\alpha = 0.5$, c = 0.4 (left) and $\alpha = 0.5$, c = 0.1 (right). In both cases $f(t) = \frac{1}{1+e^{-t}}$.

Figure 7: Comparison between the absolute error obtained by using the developed Gaussian rule (6) and the trapezoidal rule based on the double exponential transform (17) for $\alpha = 1.3$, c = 0.05 (left) and $\alpha = 0.5$, c = 0.1 (right). In both cases $f(t) = \frac{1}{1+t^2}$.

 I_n , that is,

$$p_{k+1}(t) = (t - a_k)p_k(t) - b_k p_{k-1}(t), \quad k \ge 0,$$

$$p_{-1}(t) = 0, \quad p_0(t) = 1.$$

By construction, formula (19) has the following properties (see [14]):

- 1. $\sigma_i^{(n+1)} > 0, i = 1, \dots, n+1;$
- 2. the nodes $\tau_i^{(n+1)}$ are all real and are interlaced by those of I_n ;
- 3. $\tau_i^{(n+1)} \in [0, +\infty)$, for $i \ge 2$;
- 4. $\tau_1^{(n+1)} \in [0,\infty)$ if and only if

$$\frac{p_{n+1}(0)}{p_{n-1}(0)} \ge b_{n+1}, \quad n \ge 1.$$
(21)

Let A_{2n+1}^C and A_{2n+1}^L be the generalized averaged Gaussian rules corresponding to I_n^C and I_n^L , respectively. In this way error (18) is finally estimated as

$$E_n(f) \approx \left(A_{2n+1}^C(f) - A_{2n+1}^L(f)\right) - \left(I_n^C(f) - I_n^L(f)\right).$$
(22)

In Figures 8-9 we show the reliability of the above estimate on some examples. For the Gauss-Laguerre rule I_n^L , the expressions of the corresponding orthogonal polynomials and the values of the recurrence coefficients are explicitly known. Indeed, it has been verified that (21) holds true if and only if $\alpha \ge 2$ (see [13]). As for the Gaussian formula I_n^C , since we do not have at disposal an analytical expression of the corresponding orthogonal polynomials and of the recurrence coefficients, relation (21) can only be verified numerically. The experiments show that it is not always true. Nevertheless, we remark that, even if in some cases for the rules \tilde{A}_{n+1}^C , \tilde{A}_{n+1}^L condition (21) does not hold, experimentally (for the functions considered) the resulting formulas appear to provide fairly good approximations of the quadrature error.

5 Conclusion

In this work we have considered the construction of a coupled Gaussian formula for weight functions involving powers, exponentials and oscillating functions. We have compared this new approach with the Laguerre rule and a particular double exponential trapezoidal formula. The results show that in some situations the developed rule improves the other two methods. A practical error estimate, based on the use of the generalized averaged Gaussian rule, has been presented and tested with good results.

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Figure 8: The absolute values of the error $E_n(f)$ and its estimate (22) with $\alpha = 0.7$, c = 0.5 (left) and $\alpha = 1.3$, c = 0.3. In both cases $f(t) = \frac{1}{1+t^2}$.

Figure 9: The absolute values of the error $E_n(f)$ and its estimate (22) with $\alpha = 0.5$, c = 0.4 (left) and $\alpha = 1.1$, c = 0.2. In both cases $f(t) = \frac{1}{1+e^{-t}}$.

Declaration of interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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