

# Computation and inversion of cumulative $\chi^2$ distributions

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- 2 Trigonometric and inverses
- 3 Exponential and logarithm

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5 The error function:  $\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2} dt$

6 The Airy functions: solutions of  $y''(z) - zy(z) = 0$ , particularly  
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Less elementary functions are, for instance, hypergeometric functions (Kummer, Gauss). Call them special if you wish.

Our principles for computing (special) functions:

- 1 The main objective is to develop Fortran codes which produce reliable double precision values. We don't use Maple or Mathematica in the final product.
- 2 A given special function is usually a special case of a more general function. Our approach is bottom-up: starting from the simplest cases. For example: Airy functions.
- 3 We accept that it is necessary to combine several methods in order to compute a function accurately and efficiently for a wide range of its variables.
- 4 We accept that a theoretical error analysis is usually impossible for functions with several real or complex variables. We accept more empirical approaches.
- 5 The accuracy analysis is usually done by using functional relations, such as a Wronskian relations or by comparing with an alternative method of computation.
- 6 The selection of methods in different parameter domains is based on speed and accuracy, where the latter may prevail.
- 7 Possible scaling factors may be considered when available

# A case study: Airy functions

Airy functions are the solutions of the ODE:

## The Airy equation

$$y''(z) - zy(z) = 0$$

Relatively recent methods for computing this function in the complex plane are:

- 1 Fabijonas, Lozier, Olver (ACM TOMS 2004)
- 2 Gil, Segura, Temme (ACM TOMS 2002)

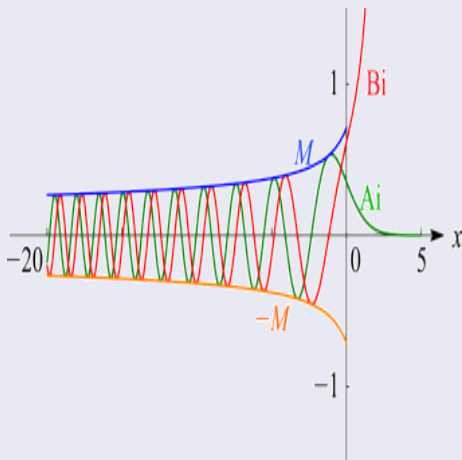
**The goal:** computing a **numerically satisfactory pair** of solutions of the Airy equation for unrestricted values of the variable (possibly factoring out an elementary function). A numerically satisfactory pair should comprise the recessive solution ( $Ai(z)$  is recessive as  $|z| \rightarrow \infty$ ,  $\arg(z) < \pi/3$ ).

I am describing briefly the case of  $Ai(z)$ , starting with positive real  $z$ .

# A case study: Airy functions

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# Convergent series

We try power series and get two independent solutions:

$$y_1(z) = \sum_{k=0}^{\infty} 3^k \left(\frac{1}{3}\right)_k \frac{z^{3k}}{(3k)!}, \quad y_2(z) = \sum_{k=0}^{\infty} 3^k \left(\frac{2}{3}\right)_k \frac{z^{3k+1}}{(3k+1)!}$$

where  $3^k(\alpha + 1/3)_k = (3\alpha + 1)(3\alpha + 4) \cdots (3\alpha + 3k - 2)$

The series converge in  $\mathbb{C}$ . Good. **Have we finished?**

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No, we haven't:  $\lim_{z \rightarrow +\infty} y_1(z) = +\infty$ ,  $\lim_{z \rightarrow +\infty} y_2(z) = +\infty$ , and we need the solution  $Ai(z)$  such that  $\lim_{z \rightarrow +\infty} Ai(z) = 0$ .

Of course, we have some  $\alpha, \beta$  such that

$$Ai(z) = \alpha y_1(z) + \beta y_2(z)$$

But this is numerically unstable for large  $x$  (we would compute a small quantity from two much larger ones)

# Divergent series

Now, we transform the equation  $y'' - zy = 0$  by considering the functions  $Y(z) = z^{1/4}y(z)$ , which, in the variable  $\zeta = 2/3z^{3/2}$ , satisfy the ODE

$$\ddot{Y}(\zeta) + \left[ -1 + \frac{5}{36\zeta^2} \right] Y(\zeta) = 0$$

This suggests that  $Y(\zeta) \sim e^{\pm\zeta}$  as  $\zeta \rightarrow +\infty$  (Liouville-Green approximation). For a better approximation, write  $Y(\zeta) = e^{-\zeta}g(\zeta)$ . Now  $g(\zeta)$  satisfies

$$\frac{d^2g}{d\zeta^2} - 2\frac{dg}{d\zeta} + \frac{\lambda}{\zeta^2}g = 0, \quad \lambda = \frac{5}{36},$$

and using a formal series in powers of  $\zeta^{-1}$ , that is,  $g(\zeta) = \sum_{k=0}^{\infty} a_m \zeta^{-m}$ , we get

$$\begin{aligned} \text{Ai}(z) &\sim z^{-1/4} e^{-\zeta} \sum_{m=0}^{\infty} a_m \zeta^{-m}, \quad \zeta = \frac{2}{3} z^{3/2}, \\ a_{m+1} &= -\frac{\lambda + m(m+1)}{2(m+1)} a_m, \quad a_0 = (2\sqrt{\pi})^{-1} \end{aligned}$$

which is a divergent series with asymptotic nature.

# Asymptotic expansions

When we say that an expansion of the form

$$f(z) \sim \sum_{n=0}^{\infty} a_n z^{-n}, \quad z \rightarrow \infty$$

is an *asymptotic expansion*, we assume that

$$z^N \left( f(z) - \sum_{n=0}^{N-1} a_n z^{-n} \right), \quad N = 0, 1, 2, \dots,$$

where the sum is empty when  $N = 0$ , is a bounded function for large values of  $z$ , with limit  $a_N$  as  $z \rightarrow \infty$ , for any  $N$ . This can also be written as

$$f(z) = \sum_{n=0}^{N-1} a_n z^{-n} + \mathcal{O}(z^{-N}), \quad z \rightarrow \infty.$$

# A first algorithm

We have two possible approximations: for  $x$  small and large. Can we match them?

- 1 Small positive  $x$  ▶ Convergent series
- 2 Large positive  $x$  ▶ Divergent series

We get  $10^{-8}$  relative precision using convergent series for  $x < 5.5$  and divergent series for  $x > 5.5$ .

For more precision, we need something else.

**We can not expect to compute a function numerically with a single method unless it is quite elementary.**

For improving the computation of Airy functions, additional approximations should be considered for intermediate  $z$ . Some possibilities:

- 1 Chebyshev expansions (for real  $x$  only)
- 2 Numerical quadrature [Gil, Segura, Temme 2002]
- 3 Numerical integration of the ODE [Fabijonas, Olver, Lozier 2004]

Let us describe the last two methods (very briefly).

# ODE integration

**Conditioning:** because  $\lim_{x \rightarrow +\infty} \text{Ai}(x)/\text{Bi}(x) = 0$ , one should never compute numerically  $\text{Ai}(x)$  integrating from  $x = 0$ .

Instead, the problem must be put this way for  $\text{Ai}(x)$ :

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Compute  $Ai(x)$  in  $[0, b]$  starting from  $Ai(b)$  and  $Ai'(b)$ . Take large  $b$ , such that  $Ai(b)$  and  $Ai'(b)$  can be approximated by asymptotics.

A possible integration method is Taylor's method:

$$y(x-h) = \sum_{n=0}^{+\infty} \frac{y^{(n)}(x)}{n!} (-h)^n$$

and the derivatives can be computed from  $y(x)$ ,  $y'(x)$  considering  $y''(x) = xy(x)$  and

$$y^{(n+2)}(x) - xy^{(n)}(x) - ny^{(n-1)}(x) = 0, \quad n \geq 1$$



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Is the application of the recurrence stable?



# Numerical quadrature

Many (special functions) can be written using integral representations, also Airy functions. Two representations are:

$$\text{Ai}(x) = \frac{1}{\pi} \int_0^{+\infty} \cos(t^3/3 + xt) dt$$

$$\text{Ai}(z) = \frac{1}{2\pi i} \int_{\infty e^{-i\pi/3}}^{+\infty e^{i\pi/3}} \exp(t^3/3 - zt) dt$$

$$\text{Ai}(z) = \frac{1}{\sqrt{\pi}(48)^{1/6}\Gamma(5/6)} e^{-\zeta} \zeta^{-1/6} \int_0^{+\infty} \left(2 + \frac{t}{\zeta}\right)^{-1/6} t^{-1/6} e^{-t} dt$$

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Which one is the best for numerical purposes?

The second one does not have an oscillating integrand and shows explicitly the dominant factor. But the first integrals can be transformed by complex integration methods (saddle point analysis).

## Numerical quadrature: a trivial example of contour deformation

$$I = \int_{-\infty}^{+\infty} \cos(w^2/2 + xw) dw = \Re(F),$$

$$F = \int_{-\infty}^{+\infty} e^{\phi(w)} dw, \quad \phi(t) = i(w^2/2 + xw)$$

$$\phi'(w_0) = 0 \rightarrow w_0 = -x$$

The path  $w = v - x + iv$ ,  $v \in (-\infty, +\infty)$  is of steepest descent (SD) and one can deform the original path to the SD path, where  $dw = (1 + i)dv$ ,  $\Re(\phi(w)) = -v^2$  and:

$$F = \int_{-\infty}^{+\infty} e^{\phi(w)} dw = e^{\phi(w_0)}(1 + i) \int_{-\infty}^{+\infty} e^{-v^2} dv$$

The remaining integral is suited for the trapezoidal rule (not needed).  
With this  $F = e^{-ix^2/2}(1 + i)\sqrt{\pi}$  and  $I = \sqrt{2\pi} \cos(x^2/2 - \pi/4)$ .

Our recipe for complex Airy functions:

- 1 MacLaurin series.
- 2 Asymptotic expansions
- 3 Gauss-Laguerre quadrature (but also the trapezoidal rule)

# Recurrence relations

Many special functions satisfy difference equations, and in particular,

$$y_{n+1} + b_n y_n + a_n y_{n-1} = 0$$

Examples:  $U(a, x)$  and  $V(a, x)$  ( $a \equiv n$ ) or  $P_{-1/2+i\tau}^m(x)$  ( $m \equiv n$ )

Recurrence relations are simple methods of computation, **if applied correctly.**

**Example:** Consider the recurrence  $y_{n+1} - y_n - y_{n-1} = 0$ , (Fibonacci) with general solution  $y_n = \alpha\phi^n + \beta(-\phi^{-1})^n$ ,  $\phi = (1 + \sqrt{5})/2$ .

Consider the numerical computation of the  $(-\phi)^{-n}$  starting from  $y_0 = 1$ ,  $y_1 = -2/(1 + \sqrt{5})$ . We compute up to  $n = 50$ .

We should get  $y_{50}/y_{49} = -2/(1 + \sqrt{5})$ , but we get  $y_{50}/y_{49} = 1.618150\dots$

The solution  $y_n = \phi^n$  dominates over  $(-\phi^{-1})^n$  (minimal). Any small numerical error introduces the dominant solution. This is a conditioning problem; **we need information on the conditioning of the solutions.**



## Recurrences: main results to be considered

- 1 Perron-Kreuser theorem, which essentially says that for a linear difference equation of order  $k$ ,  $y_{n+k+1} + a_n^{(n+k)} y_{n+k} + \dots + a_n^{(0)} y_n = 0$  there exist different solutions such the ratios  $y_{n+1}/y_n$  behave as  $n \rightarrow +\infty$  as the solutions of the characteristic equation  $\lambda^{n+k+1} + a_n^{(n+k)} \lambda^{n+k} + \dots + a_n^{(0)} = 0$  (in the non-degenerate case).
- 2 The asymptotic behavior of the solution we want to compute, to be compared with the Perron-Kreuser predictions. Is the solution recessive (minimal), dominant or none of them?
- 3 Pincherle's theorem for three term recurrence relations:  
 $y_{n+1} + b_n y_n + a_n y_{n-1} = 0$  has minimal solution  $\{f_n\}$  if and only if:

$$\frac{f_n}{f_{n-1}} = \frac{-a_n}{b_n + \frac{-a_{n+1}}{b_{n+1} + \dots}}$$

## Additional examples of computation

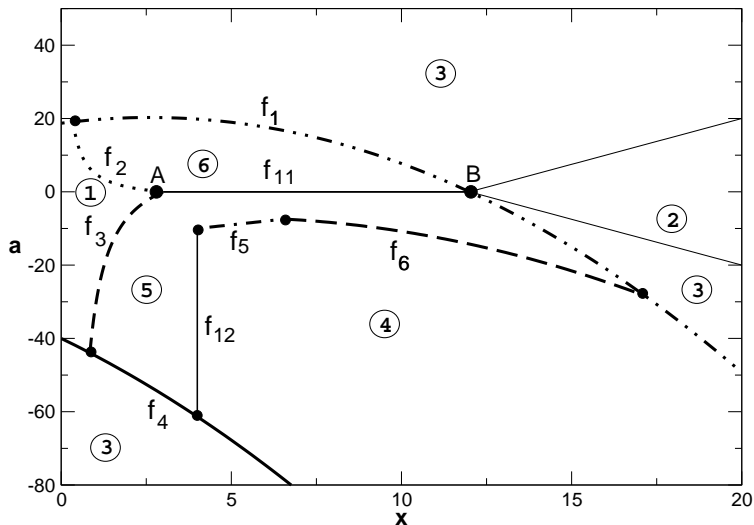
We have solved some other problems, like:

- 1 Various types of Legendre functions of real parameters.
- 2 Inhomogeneous Airy functions.
- 3 Solution of the Bessel equation  $x^2 y'' + xy + (x^2 + a^2)y = 0$  (2004). Numerically satisfactory pair  $\{K_{ia}(x), L_{ia}(x)\}$ .
- 4 Solution of the parabolic cylinder equation  $y'' + (a \pm x^2/4)y = 0$  (2006 for  $-$ , 2011 and 2012 for  $+$ ). Pairs of solutions  $\{U(a, x), V(a, x)\}$  ( $-$  case) and  $\{W(a, x), W(a, -x)\}$
- 5 Conical functions, that is, Legendre functions  $P_{-1/2+ir}^m(x)$  (2009, 2012).
- 6 Incomplete gamma functions  $\gamma(a, x), \Gamma(a, x)$  (2012)

The last four problems are harder because they involve two or more variables. A good number of methods are usually needed to cover a large range.



Case of the parabolic cylinder equation (–):



# Computation of $\chi^2$ cumulative distributions

Recent activity involves the computation of inversion of  $\chi^2$  cumulative distributions.

The central distributions are given by the incomplete gamma function ratios

$$P(a, x) = \frac{1}{\Gamma(a)} \int_0^x t^{a-1} e^{-t} dt, \quad Q(a, x) = \frac{1}{\Gamma(a)} \int_x^{+\infty} t^{a-1} e^{-t} dt$$

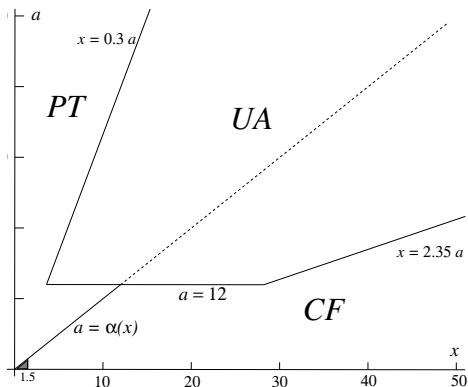
Because  $P(a, x) + Q(a, x) = 1$  we only need to compute one function. We compute the smallest of the two.

For large values of  $a, x$  we have a transition at  $a \sim x$ , with

$$P(a, x) \lesssim \frac{1}{2} \quad \text{when} \quad a \gtrsim x,$$

$$Q(a, x) \lesssim \frac{1}{2} \quad \text{when} \quad a \lesssim x.$$

Accordingly, the methods of computation are divided in two zones, with several methods of computation in each one.



PT: Taylor series for  $P$

QT: Taylor series for  $Q$  (small triangle)

UA: Uniform asymptotic expansions (Temme, 1979)

CF: continued fraction for the  $Q$  (Gautschi, 1977)

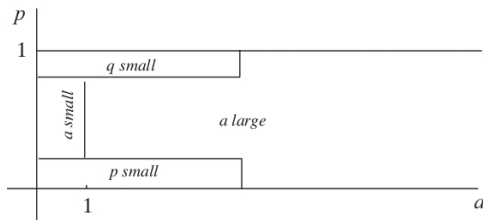
## Inversion of the cumulative central $\chi^2$ distribution

For probability distributions, the inversion is also needed in applications. For fixed  $a$ , we invert  $P(a, x) = p$  or, equivalently,  $Q(a, x) = q$ .

Our approach:

- 1 Invert  $P(a, x)$  ( $Q(a, x)$ ) if  $p < q$  ( $p > q$ )
- 2 Use the existent approximation methods (PT, Poincaré asymptotics for  $Q$ , UA) to find starting values.
- 3 Apply higher order Newton methods from the resulting starting values.

The different type of starting values are chosen according to the next figure.



An example of inversion:

For small  $p$ , we use PT to write

$$x = r \left( 1 + \sum_{n=1}^{\infty} \frac{a(-1)^n x^n}{(a+n)n!} \right)^{-1/a}, \quad r = (p\Gamma(1+a))^{1/a},$$

We write  $x = r + \sum_{n=2}^{\infty} c_k r^k$ , and by expanding the first few coefficients are

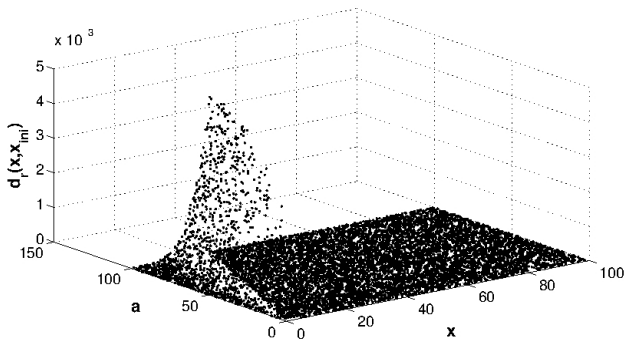
$$c_2 = \frac{1}{a+1},$$

$$c_3 = \frac{3a+5}{2(a+1)^2(a+2)},$$

$$c_4 = \frac{8a^2 + 33a + 31}{3(a+1)^3(a+2)(a+3)},$$

$$c_5 = \frac{125a^4 + 1179a^3 + 3971a^2 + 5661a + 2888}{24(1+a)^4(a+2)^2(a+3)(a+4)}.$$

The accuracy of the starting values (except for small  $a$ ) is shown in this figure



With a fourth order Newton-like method, 2 or 3 iterations are enough for an accuracy better than  $10^{-12}$ .

## The Marcum Q-function

The generalized Marcum Q-function is the **non-central cumulative  $\chi^2$  distribution**, up to elementary redefinition of the variables. It is defined as

$$Q_{\mu}(x, y) = x^{\frac{1}{2}(1-\mu)} \int_y^{+\infty} t^{\frac{1}{2}(\mu-1)} e^{-t-x} I_{\mu-1}(2\sqrt{xt}) dt,$$

where  $\mu > 0$  and  $I_{\mu}(z)$  is the modified Bessel function. For  $\mu = 1$  the function is known as the Marcum Q-function.

We also use a complementary function such that  $P_{\mu}(x, y) + Q_{\mu}(x, y) = 1$  :

$$P_{\mu}(x, y) = x^{\frac{1}{2}(1-\mu)} \int_0^y t^{\frac{1}{2}(\mu-1)} e^{-t-x} I_{\mu-1}(2\sqrt{xt}) dt.$$

Particular values are

$$Q_{\mu}(x, 0) = 1, \quad Q_{\mu}(x, +\infty) = 0,$$

$$Q_{\mu}(0, y) = Q_{\mu}(y), \quad Q_{\mu}(+\infty, y) = 1,$$

$$Q_{+\infty}(x, y) = 1.$$

As for incomplete gamma functions, we compute the smallest of the two functions. Asymptotic analysis gives that for large values of  $\mu, x, y$ , we have a transition at  $y \sim x + \mu$ , with

$$P_{\mu}(x, y) \lesssim Q_{\mu}(x, y) \quad \text{when} \quad y \lesssim x + \mu,$$

$$Q_{\mu}(x, y) \lesssim P_{\mu}(x, y) \quad \text{when} \quad y \gtrsim x + \mu.$$

Ingredients in the computation:

- 1 Series in terms of incomplete gamma functions
- 2 Recurrence relations.
- 3 Asymptotic expansions for large  $\mu$  in terms of the error function (both for  $P$  and  $Q$ ).
- 4 Quadrature methods.

We give some details of these methods.



# Series in incomplete gamma functions

Plugging the Maclaurin series for the modified Bessel function into the integral representation, we readily obtain the series expansions

$$P_\mu(x, y) = e^{-x} \sum_{n=0}^{\infty} \frac{x^n}{n!} P_{\mu+n}(y),$$

$$Q_\mu(x, y) = e^{-x} \sum_{n=0}^{\infty} \frac{x^n}{n!} Q_{\mu+n}(y).$$

in terms of the incomplete gamma function ratios (which we can compute). Recurrences can be used to compute rapidly the series. We have

$$Q_{\mu+1}(y) = Q_\mu(y) + \frac{y^\mu e^{-y}}{\Gamma(\mu + 1)},$$

$$P_{\mu+1}(y) = P_\mu(y) - \frac{y^\mu e^{-y}}{\Gamma(\mu + 1)},$$

stable for  $Q_\mu(y)$  in the forward direction, and for  $P_\mu(y)$  in the backward direction. Equivalently, we have  $\mu Q_{\mu+1}(y) - (\mu + y)Q_\mu(y) + yQ_{\mu-1}(y) = 0$ .

The series

$$Q_\mu(x, y) = e^{-x} \sum_{n=0}^{\infty} \frac{x^n}{n!} Q_{\mu+n}(y)$$

can be computed from two values  $Q_\mu(y)$  and  $Q_{\mu+1}(y)$  and forward recursion with

$$Q_{\mu+1}(y) = \left(1 + \frac{y}{\mu}\right) Q_\mu(y) - \frac{y}{\mu} Q_{\mu-1}(y)$$

For the other series, we write

$$P_\mu(x, y) \simeq e^{-x} P_\mu(y) \sum_{n=0}^{n_0} \frac{x^n}{n!} \frac{P_{\mu+n}(y)}{P_\mu(y)},$$

estimate the value  $n_0$  which gives sufficient accuracy and compute using the backward recursion

$$Q_{\mu-1}(y) = -\frac{\mu}{y} Q_{\mu+1}(y) + \left(1 + \frac{\mu}{y}\right) Q_\mu(y)$$

# Recurrence relations

Integration by parts gives the following recurrences

$$Q_{\mu+1}(x, y) = Q_{\mu}(x, y) + \left(\frac{y}{x}\right)^{\mu/2} e^{-x-y} I_{\mu}(2\sqrt{xy}),$$

$$P_{\mu+1}(x, y) = P_{\mu}(x, y) - \left(\frac{y}{x}\right)^{\mu/2} e^{-x-y} I_{\mu}(2\sqrt{xy}),$$

It is possible to eliminate the Bessel function and obtain a homogeneous third order recurrence relation.

$$xQ_{\mu+2}(x, y) = (x - \mu)Q_{\mu+1}(x, y) + (y + \mu)Q_{\mu}(x, y) - yQ_{\mu-1}(x, y),$$

and  $P_{\mu}(x, y)$  satisfies the same relation, but its computation with this recurrence is badly conditioned (it is subdominant, but not minimal)

A better possibility is:

$$y_{\mu+1} - (1 + c_{\mu})y_{\mu} + c_{\mu}y_{\mu-1} = 0, \quad c_{\mu} = \sqrt{\frac{y}{x}} \frac{I_{\mu}(2\sqrt{xy})}{I_{\mu-1}(2\sqrt{xy})}.$$

$P$  is minimal and  $Q$  is dominant. Pincherle's theorem gives:

$$\frac{P_{\mu}(x, y)}{P_{\mu-1}(x, y)} = \frac{c_{\mu}}{1 + c_{\mu}} - \frac{c_{\mu+1}}{1 + c_{\mu+1}} - \dots$$

# Asymptotic expansions

We start from

$$Q_{\mu+1}(\mu x, \mu y) = \frac{\mu e^{-\mu x}}{(2x)^{\mu+1}} \int_{\xi}^{\infty} z e^{-\mu \phi(z)} e^{-\mu \eta(z)} I_{\mu}(\mu z) dz,$$

where

$$\phi(z) = -\ln z + \frac{1}{4x} z^2 - \eta(z), \quad \eta(z) = \sqrt{1+z^2} + \log \frac{z}{1+\sqrt{1+z^2}}, \quad \xi = 2\sqrt{xy}$$

The saddle point follows from the equation  $\phi'(z) = 0$ . It follows that the positive saddle point  $z_0$  is given by

$$z_0 = 2\sqrt{x(1+x)}. \quad (1)$$

The transition line in the scaled variables is  $y = x + 1$ .

The saddle point coalesces with the end point of integration as  $y \rightarrow x + 1$ . Bleistein's method is a good choice (we omit details).

$Q$  is computed for  $y > x + 1$  (in the unscaled variables  $y > x + \mu$ ).

For  $P$  analogous expansions can be worked out ( $y < x + \mu$ )



$$Q_{\mu}(\mu x, \mu y) \sim \frac{1}{2} \operatorname{erfc}\left(-\zeta \sqrt{\mu/2}\right) + \sqrt{\frac{\mu}{2\pi}} \sum_{k=1}^{\infty} B_k - e^{-\frac{1}{2}\mu\zeta^2} e^{-\mu\eta(\zeta)} I_{\mu}(\mu\xi).$$

$$B_k = \sum_{j=0}^k \frac{f_{j,k-j} \Psi_j(\zeta)}{\mu^{k-j}}$$

$$\Psi_j(\zeta) = \left(\frac{2}{\mu}\right)^{(j+1)/2} \int_{-\zeta\sqrt{\mu/2}}^{\infty} e^{-s^2} s^j ds.$$

which can be written in terms of incomplete gamma functions.

$$\zeta = \operatorname{sign}(x+1-y) \sqrt{2(\phi(\xi) - \phi(z_0))}.$$

$$f_k(w) = \frac{z}{2x} \frac{u_k(t)}{(1+z^2)^{\frac{1}{4}}} \frac{dz}{dw} = \sum_{j=0}^{\infty} f_{jk} (w - \zeta)^j, \quad t = 1/\sqrt{1+z^2}$$

$$\phi(z) - \phi(\xi) = \frac{1}{2} w^2 - \zeta w, \quad \xi = 2\sqrt{xy}$$

$$u_0(t) = 1, \quad u_1(t) = \frac{3t - 5t^3}{24}, \quad u_2(t) = \frac{81t^2 - 462t^4 + 385t^6}{1152},$$

and other coefficients can be obtained by applying the formula

$$u_{k+1}(t) = \frac{1}{2} t^2 (1 - t^2) u_k'(t) + \frac{1}{8} \int_0^t (1 - 5s^2) u_k(s) ds, \quad k = 0, 1, 2, \dots$$

# Numerical quadrature

Starting point:

$$Q_{\mu}(\mu X, \mu Y) = \frac{e^{-\mu(x+y)}}{2\pi i} \int_{\mathcal{L}_Q} \frac{e^{\mu\phi(s)}}{1-s} ds,$$

where  $\mathcal{L}_Q$  is a vertical line that cuts the real axis in a point  $s_0$ , with  $0 < s_0 < 1$ , and

$$\phi(s) = \frac{x}{s} + ys - \ln s.$$

A similar representation can be obtained for  $P$ .

The contour is deformed in such a way that it passes through the saddle point of  $\phi$ , similarly as we did in our simple example and then the trapezoidal rule is used.

We omit details.

The methods are combined as follows:

Let  $f_1(x, \mu) = x + \mu - 0.25\sqrt{4x + 2\mu}$ ,  $f_2(x, \mu) = x + \mu + 0.25\sqrt{4x + 2\mu}$ .

- 1 If  $\mu > 60$ , compute the Marcum functions using either with asymptotic expansions for  $f_1(x, \mu) < y < f_2(x, \mu)$  and use numerical quadrature in the other case.
- 2 If  $\mu \leq 60$ , compute the Marcum functions as follows:
  - If  $\mu \leq 10$ ,  $x < 15$ ,  $y < 15$ , compute the series expansion.
  - In other case: if  $y < f_1(x, \mu)$  or  $y > f_2(x, \mu)$  compute by numerical quadrature; if  $f_1(x, \mu) < y < f_2(x, \mu)$  compute the Marcum functions using the recurrence relation.

The algorithm has been implemented in a Fortran 90 module **MarcumQ**, which includes the Fortran 90 routine **marcum** for the computation of  $Q_\mu(x, y)$  and  $P_\mu(x, y)$ . We have tested that an accuracy  $\sim 10^{-12}$  can be obtained in the parameter region  $(x, y, \mu) \in [0, 200] \times [0, 200] \times [1, 200]$  (submitted to ACM Trans. Math. Softw.)

# Inversion of the Marcum Q-function

For a three variable function, we have to fix what we mean by inversion. It appears that in applications the inversion process is as follows (Helstrom, 1998):

We are given two numbers  $q_0, q_1$ , both in  $(0, 1)$ , and we assume a fixed value of  $m$ .

**Step 1:** Find  $y$  from the equation

$$Q_\mu(0, y) = q_0,$$

and denote this value with  $y_0$ . Because  $Q_\mu(0, y) = Q_\mu(y)$  (the normalized incomplete gamma function) we already know how to do this step.

**Step 2:** Find  $x$  from the equation

$$Q_\mu(x, y_0) = q_1, \quad (2)$$

and denote this value with  $x_1$ . The value  $y_0$  is obtained in Step 1.

Work in progress



Next steps:

- 1 Consider asymptotic inversion (large  $\mu$ ). **Nearly done.**
- 2 Analyze the converge of Newton-like methods, not only for large  $\mu$ .
- 3 About direct computation: should we consider a generalization of Marcum-Q?

Nutall function:

$$Q_{\eta,\mu}(x, y) = x^{\frac{1}{2}(1-\mu)} \int_y^{+\infty} t^{\eta+\frac{1}{2}(\mu-1)} e^{-t-x} I_{\mu-1}(2\sqrt{xt}) dt,$$

$$Q_{0,\mu}(x, y) = Q_{\mu}(x, y)$$

Or should we go back to hypergeometric functions? We will see...

Thank you!