# Recent software developments for special functions in the Santander-Amsterdam project

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# Keywords

- Algorithms for special functions
- Power series, asymptotic expansions
- Recurrence relations
- Uniform asymptotic expansions
- Numerical quadrature
- Continued fractions
- Inversion of distribution functions
- Incomplete gamma functions
- Marcum's $Q-$function, noncentral $\chi^2$

# Project Santander-Amsterdam

- First email contact: 3 September 1997
- First personal contact: SIAM Annual Meeting 1998 Toronto
- Lecture by Bruce Fabijonas on Scorer functions motivated research in contour integrals for these functions.
- The project has been supported with a number of grants from *Ministerio de Ciencia e Innovación*

# Publications and algorithms

- 27 published papers, from 2000,
- of which 5 Algorithms in ACM TOMS
- and 3 Algorithms in CPC (all in FORTRAN 90)
- 1 submitted paper, 1 in preparation

# Publications and algorithms

Special publications:

- 1 book: *Numerical methods for Special Functions*
- 1 survey paper (2007) in *Acta Numerica*
- 1 survey paper (2011) in *Recent Advances in Computational and Applied Mathematics*, Simos (ed.), Springer
- 1 survey paper (2012) in *Encyclopedia of Applied and Computational Mathematics*, Engquist/Iserles (eds.), Springer
- Contributions to the  *NIST Handbook of Mathematical Functions*

# Published algorithms

- Zeros of Bessel functions
- Toroidal functions
- Complex Airy and Scorer functions
- Modified Bessel functions of imaginary order
- Real Parabolic Cylinder Functions $U, V$
- Parabolic cylinder function $W, W'$
- Conical function $P^{m}_{-1/2+i\tau}(x)$
- Regular and irregular associated Legendre functions

# Pre-project published algorithms

Amparo & Javier: several algorithms in CPC

- Modified Bessel functions, continued fraction method
- Zeros of Bessel functions
- Prolate and oblate spheroidal harmonics
- Parabolic cylinder functions of integer and half-integer orders
- A Monte Carlo code to simulate 3D buffered diffusion
- Toroidal harmonics
- Legendre functions of argument greater than one

# Numerical topics, methods

Publications on

- Zeros of Scorer and other special functions
- Recurrence relations for hypergeometric functions (Gauss and Kummer)
- Contour integral representations of PCF's
- Quadrature methods for contour integrals
- Inversion of cumulative distribution functions
- Computation and inversion of incomplete gamma functions and the Marcum $Q-$function

# Details on numerical methods

We give a few comments on the following basic methods:

- Series expansions; convergent, asymptotic
- Recurrence relations
- Quadrature methods

First: our way of working (paradigms?).

# Details on numerical methods

Our main principles:

1. Generalize or not ?

   A given special function is usually a special case of a more general function. Keep it simple.
2. Error analysis or not ?

   For a function with several (complex) variables, detailed error analysis is usually impossible.
3. How to verify the result ?

   For a start: Maple. At the end: functional relations.
4. Which method to use ?

   Series, recursions, integrals; all with stable representations.
5. Parameter domain ?

   Also large or complex parameters. Use scaling.

# Details on numerical methods
# Generalize or not ?

Start with ${}_pF_q(a_1,\ldots,a_p;b_1,\ldots,b_q;z)$ or with the Meijer $G-$function

$$G^{m,n}_{p,q}(z;\mathbf{a};\mathbf{b}) = G^{m,n}_{p,q}\left(z;\, {a_1,\ldots,a_p \atop b_1,\ldots,b_q}\right) =$$

$$\frac{1}{2\pi i}\int_{\mathcal{L}} \frac{\prod_{\ell=1}^{m}\Gamma(b_\ell - s)\prod_{\ell=1}^{n}\Gamma(1-a_\ell+s)}{\prod_{\ell=m}^{q-1}\Gamma(1-b_{\ell+1}+s)\prod_{\ell=n}^{p-1}\Gamma(a_{\ell+1}-s)} z^s\,\mathrm{d}s\,?$$

Here the integration path $\mathcal{L}$ separates the poles of the factors $\Gamma(b_\ell - s)$ from those of the factors $\Gamma(1-a_\ell+s)$.

# Details on numerical methods
# Generalize or not ?

A Meijer $G-$function can be written as a finite sum of ${}_pF_q-$functions.

These functions can be computed by using their power series or large $z$ asymptotic expansions.

Example: modified Bessel function

$$K_\nu(z) = \tfrac{1}{2}\pi \frac{I_{-\nu}(z) - I_\nu(z)}{\sin(\nu\pi)}.$$

This is the approach in SAGE for $G-$functions, and perhaps in other computer algebra packages.

Case closed?

# Details on numerical methods
# Generalize or not ?

There are two main problems

1. Representation for positive large $\Re z$:
   - The function $I_\nu(z)$ is exponentially large.
   - The function $K_\nu(z)$ is exponentially small.

   This can be controlled by including more and more digits in the computations.

2. For integer $\nu$, the relation between $K_\nu(z)$ and $I_\nu(z)$ is well-defined analytically, but it becomes useless for numerical computations.

   This is difficult to handle, even in computer algebra packages.

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# Details on numerical methods

Series expansions; convergent, asymptotic

- Simple for implementation
- Be careful with stopping criteria
- Bridge the gap: convergent $\Leftrightarrow$ asymptotic
- For this:
  - continued fractions,
  - quadrature methods,
  - $\ldots$

# Details on numerical methods

Recurrence relations:

$$A_n y_{n-1} + B_n y_n + C_n y_{n+1} = 0$$

- Theory: Poincaré, Perron, Kreuser, . . .
- Minimal $f_n$, dominant $g_n$ solutions if

$$\lim_{n\to\infty} \frac{f_n}{g_n} = 0$$

- Use backward recursion for $f_n$ (Miller, Olver, . . . )
- Use continued fraction methods for $f_n$
- Warning: anomalous convergence may happen because of the role of other (than $n$) parameters

# Details on numerical methods

Quadrature methods:

- The standard integral representations may be not convenient: oscillations, bad convergence, . . .
- Use complex contour integrals through saddle points
- Use simple quadrature rule: trapezoidal
- Take out dominant factor for scaling

# How to compute this integral ?

Consider

$$F(\lambda) = \int_{-\infty}^{\infty} e^{-t^2+2i\lambda\sqrt{t^2+1}}\, \mathrm{d}t.$$

- Maple 14, for $\lambda = 10$, gives

$$F(10) = -.1837516481 + .5305342893i.$$

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- So, the first answer seems to be correct in all shown digits.

# How to compute this integral ?

Take another integral, which is almost the same:

$$F(\lambda) = \int_{-\infty}^{\infty} e^{-t^2+2i\lambda\sqrt{t^2+1}}\, \mathrm{d}t \Longrightarrow G(\lambda) = \int_{-\infty}^{\infty} e^{-t^2+2i\lambda t}\, \mathrm{d}t.$$

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- The correct answer is $G(10) = 0.6593662989 \times 10^{-43}$.

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- The correct answer is $G(10) = 0.6593662989 \times 10^{-43}$.
- Maple 14, with procedure *int*, gives $G(10) = e^{-100}\sqrt{\pi}$.

# How to compute this integral ?

The message is: one should have some feeling about the computed result.

Otherwise a completely incorrect answer can be accepted.

Mathematica 7 is more reliable here, and gives a warning with answer $0. \times 10^{-16} + 0. \times 10^{-17} i$.

# Incomplete gamma ratios

For $x > 0, a > 0$:

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

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

with

$$P(a,x) + Q(a,x) = 1.$$

Compute first $\min(P,Q)$, then the other one.

# Incomplete gamma ratios

Many tools are available:

- Recursion; not used
- Series; convergent, asymptotic
- Continued fractions
- Uniform asymptotic expansions
- Simple or contour integrals; not used

Motivation: inversion methods; Marcum $Q$.

Main source: Gautschi (1979), who used a different domain (also $a < 0$) and a different pair of functions (different scaling of $P$ and $Q$).

# Incomplete gamma ratios

Taylor expansions:

$$P(a,x) = \frac{x^a e^{-x}}{\Gamma(a+1)} \sum_{n=0}^{\infty} \frac{x^n}{(a+1)_n},$$

where

$$(a)_n = a(a+1)\cdots(a+n-1) = \frac{\Gamma(a+n)}{\Gamma(a)}, \quad n = 0, 1, 2, \ldots$$

Also, for $0 < x < 1.5$, $x > a$,

$$Q(a,x) = 1 - \frac{x^a}{\Gamma(a+1)} - \frac{x^a}{\Gamma(a)} \sum_{n=1}^{\infty} \frac{(-1)^n x^n}{(a+n)n!}.$$

# Incomplete gamma ratios

The tricky terms for small $x$ and $a$:

$$1 - \frac{x^a}{\Gamma(a+1)} = 1 - \frac{1}{\Gamma(a+1)} + \frac{1-x^a}{\Gamma(a+1)}.$$

We write

$$1 - \frac{1}{\Gamma(a+1)} = a(1-a)g(a),$$

and provide an algorithm for $g(a)$.

And $1 - x^a = 1 - e^{a \ln x}$ can be expanded.

# Incomplete gamma ratios

Continued fraction:

$$Q(a,x) = \frac{x^a e^{-x}}{(x+1-a)\Gamma(a)} \left( \frac{1}{1+} \, \frac{a_1}{1+} \, \frac{a_2}{1+} \, \frac{a_3}{1+} \, \frac{a_4}{1+} \, \cdots \right),$$

where

$$a_k = \frac{k(a-k)}{(x+2k-1-a)(x+2k+1-a)}, \qquad k \geq 1.$$

This fraction is very useful for $x \geq 1.5$ and $x > a$, although for large $x \sim a$ we took a different approach.

# Incomplete gamma ratios

Uniform expansion:

$$Q(a,x) = \tfrac{1}{2}\,\mathrm{erfc}(\eta\sqrt{a/2}) + R_a(\eta),$$

$$P(a,x) = \tfrac{1}{2}\,\mathrm{erfc}(-\eta\sqrt{a/2}) - R_a(\eta),$$

where

$$\mathrm{erfc}\,x = \frac{2}{\sqrt{\pi}}\int_x^\infty e^{-t^2}\,dt,$$

and

$$R_a(\eta) = \frac{e^{-\frac{1}{2}a\eta^2}}{\sqrt{2\pi a}}S_a(\eta), \quad S_a(\eta) \sim \sum_{n=0}^{\infty}\frac{C_n(\eta)}{a^n},$$

# Incomplete gamma ratios

where

$$\eta = (\lambda - 1)\sqrt{\frac{2(\lambda - 1 - \ln\lambda)}{(\lambda - 1)^2}}, \qquad \lambda = \frac{x}{a},$$

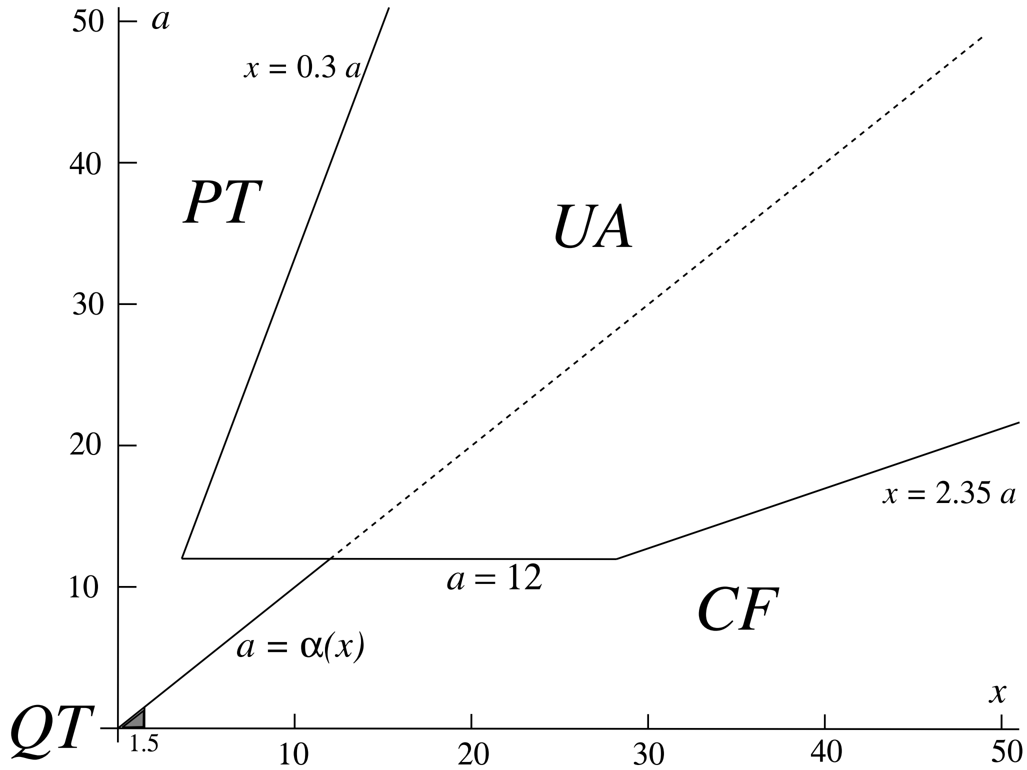
and

$$C_0(\eta) = \frac{1}{\lambda - 1} - \frac{1}{\eta} = -\tfrac{1}{3} + \tfrac{1}{12}\eta + \ldots\, .$$

Other $C_n(\eta)$ follow from a recurrence relation.

Evaluation of these coefficients when $\lambda \sim 1$ is tricky; a different approach is used for that case.

# Incomplete gamma ratios




***PT***: Taylor series for $P(a,x)$

***QT***: Taylor series for $Q(a,x)$

***CF***: continued fraction for $Q(a,x)$

***UA***: uniform method for $\min(P,Q)$

# Incomplete gamma ratios

Testing: we used the recurrence relations

$$P(a+1,x) = P(a,x) - D(a,x), \quad Q(a+1,x) = Q(a,x) + D(a,x),$$

where

$$D(a,x) = \frac{x^a e^{-x}}{\Gamma(a+1)}.$$

For large values of $a$ and $x$ we can use a scaled version:

$$p(a,x) = P(a,x)/D(a,x), \quad q(a,x) = Q(a,x)/D(a,x),$$

and these functions satisfy the recursion

$$\frac{x}{a+1} p(a+1,x) = p(a,x) - 1, \quad \frac{x}{a+1} q(a+1,x) = q(a,x) + 1.$$

# Incomplete gamma ratios

The maximum relative errors for the first recursions using $10^6$ and $10^7$ random points for two regions of the $(x, a)$-plane:

1. $(0, 1] \times (0, 1]$: $1.7\,10^{-15}$,
2. $(0, 500] \times (0, 500]$: $1.9\,10^{-13}$.

The use of the scaled recursion with $10^7$ and $10^8$ random points for two regions of the $(x, a)$-plane (excluding the UA region) gives maximum relative errors:

1. $(0, 10^4] \times (0, 10^4]$: $8.3\,10^{-15}$,
2. $(0, 10^5] \times (0, 10^5]$: $9.1\,10^{-15}$.

With $10^7$ random points in the region $(0, 10^4] \times (0, 10^4]$ , the maximum relative error obtained in the UA region is $4.0\,10^{-14}$.

# Inversion of $P(a,x), Q(a,x)$

Inversion of the equations

$$P(a,x) = p, \quad Q(a,x) = q$$

with $a$, $p$, $q$ given, $p+q=1$.

In the algorithm we request both $p$ and $q$.

If $p \le q$ then try to find $x(p,a)$ else try to find $x(q,a)$.

Use analytic estimates obtained from several representations to start a safe Newton or other process.

# Inversion of $P(a,x), Q(a,x)$

When $a$ is large we start with

$$P(a,x) \sim \tfrac{1}{2}\,\mathrm{erfc}(-\eta\sqrt{a/2}) = p,$$

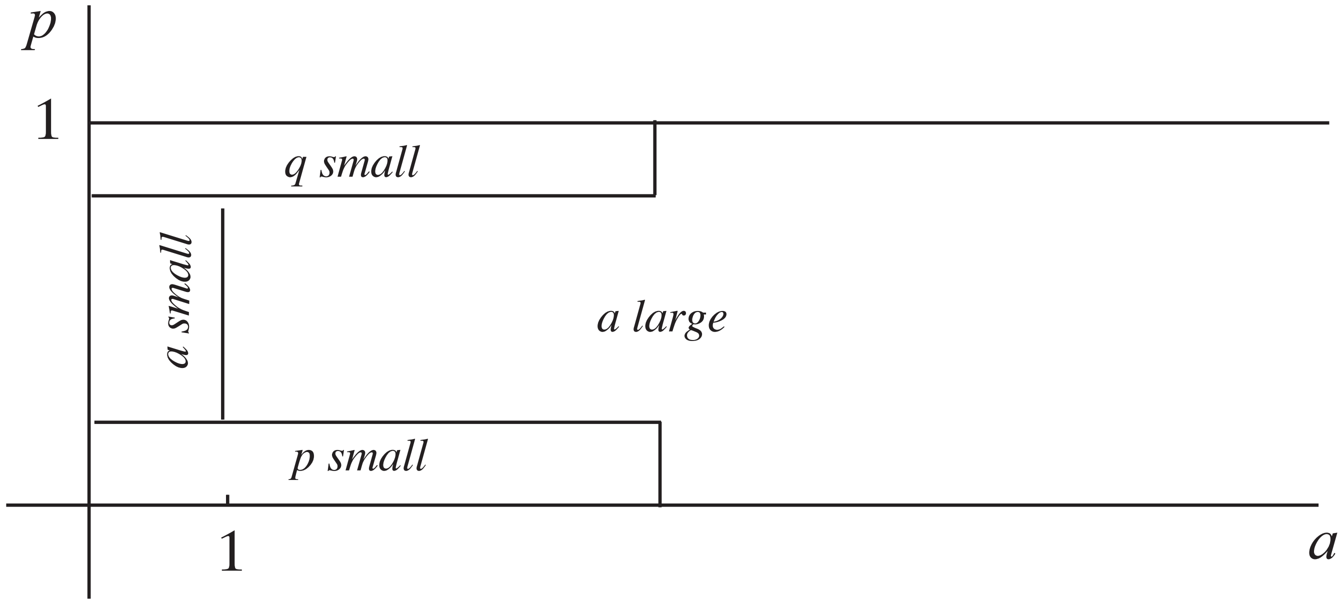
giving a starting value $\eta_0(p,a)$, and we can expand

$$\eta \sim \eta_0 + \frac{\varepsilon_1(\eta_0,a)}{a} + \frac{\varepsilon_2(\eta_0,a)}{a^2} + \frac{\varepsilon_3(\eta_0,a)}{a^3} + \ldots .$$

The first $\varepsilon_j$ can be computed easily.

This method can be used for $a \geq 1$; this means, the approximated is a reliable starting value for a few Newton steps.

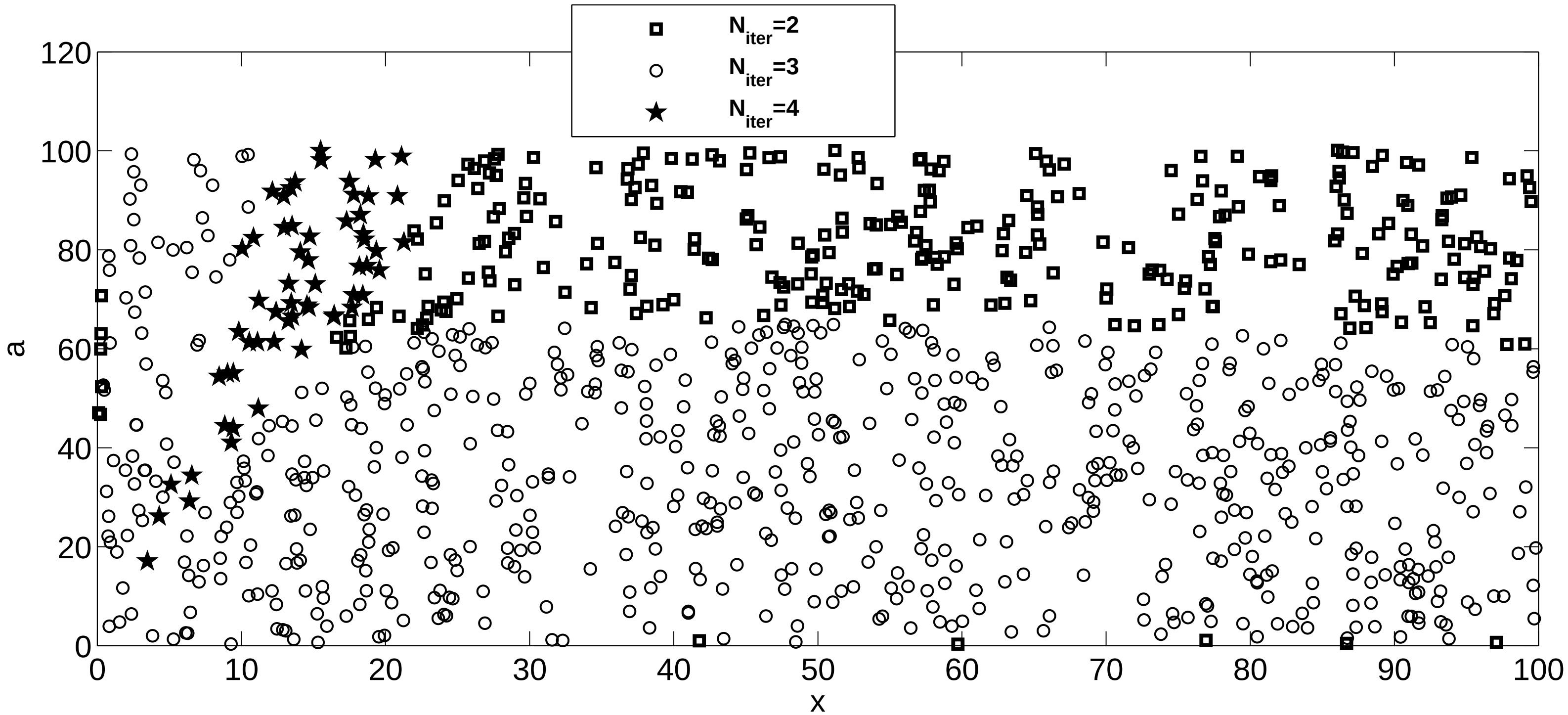
# Inversion of $P(a,x), Q(a,x)$




There are several cases which are schematically indicated here.

The algorithms improve both the accuracy and ranges of those in DiDonato & Morris (1986).

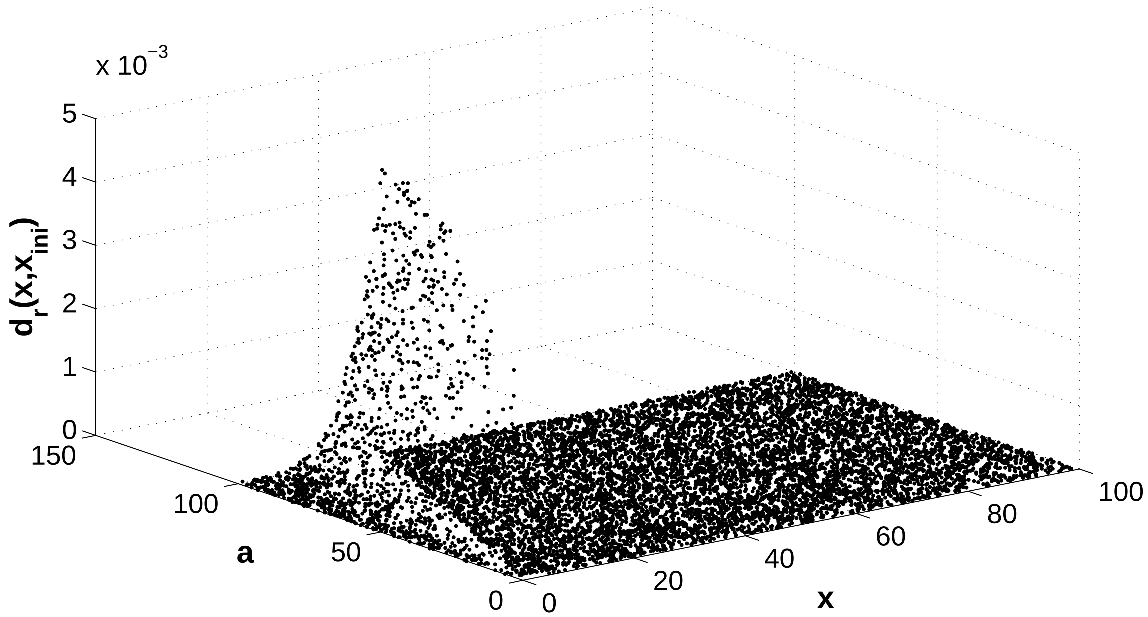
# Inversion of $P(a,x), Q(a,x)$




Number of Newton iterations used in the inversion algorithm in the region $(x, a) \in (0, 100] \times (0, 100]$.

Usually, 2 or 3 iterations are enough here.

# Inversion of $P(a,x), Q(a,x)$




Accuracy of the initial estimates: points correspond to relative distances $d_r(x, x_{ini}) = \|1 - x_{ini}/x\|$, with $x_{ini}$ the initial estimate, $x$ the true value.

Larger $x$ give better results. Also, the poorest estimate is located at a relative distance less than $5.0\,10^{-3}$ to the real value.

# Marcum's $Q-$function

Definition in terms of the modified Bessel function:

$$Q_\mu(x,y) = \int_y^\infty \left(\frac{z}{x}\right)^{\frac{1}{2}(\mu-1)} e^{-z-x} I_{\mu-1}(2\sqrt{xz})\, dz.$$

The complementary function is needed in computations:

$$P_\mu(x,y) = \int_0^y \left(\frac{z}{x}\right)^{\frac{1}{2}(\mu-1)} e^{-z-x} I_{\mu-1}(2\sqrt{xz})\, dz,$$

with $P_\mu(x,y) + Q_\mu(x,y) = 1$.

# Marcum's $Q-$function

By expanding the Bessel function:

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

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

in terms of the incomplete gamma functions. In this way, these functions are called noncentral $\chi^2$-distributions

These and several other relations motivated us to start with $P(a,x)$ and $Q(a,x)$.

# Marcum's $Q$—function

Asymptotic analysis shows a transition when $y$ passes the value $x+\mu$. There is a fast transition from 0 to 1. In fact we have for large parameters $x, y$:

$$Q_\mu(x,y) \sim \begin{cases} 1 & \text{if } x+\mu > y, \\ \frac{1}{2} & \text{if } x+\mu = y, \\ 0 & \text{if } x+\mu < y, \end{cases}$$

and complementary behaviour for $P_\mu(x,y) = 1 - Q_\mu(x,y)$.

Uniform asymptotic expansions include again $\operatorname{erfc} x$.

# Marcum's $Q$−function

Tools for computation:

- Recursions
- Series; convergent, asymptotic
- Uniform asymptotic expansions

Work in progress.

# Congratulations!