Computing infinite range integrals of an arbitrary product of Bessel functions

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Outline

Introduction

Algorithm

Finite range integration

Infinite range approximation

Optimization

Implementation issues

Cost parameter t_{GJ}

Backward compatibility

Examples

The SIAM 100-Digit Challenge

- 10 problems in high-accuracy numerical computing
- Book by winning teams Bornemann, Laurie, Wagon and Waldvogel
- Appendix D. More Problems.

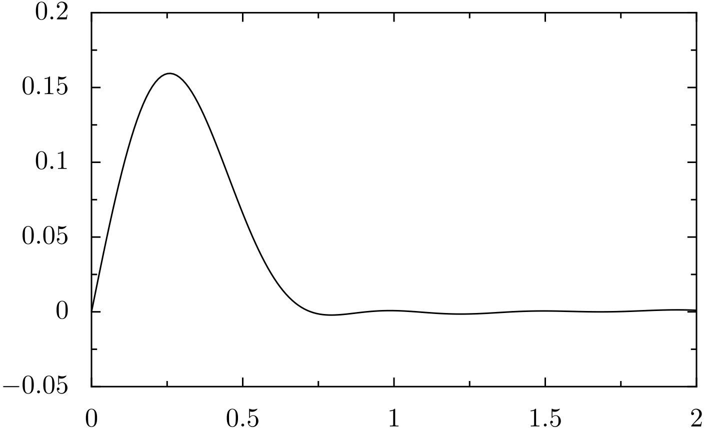
Problem 8

What is the value of

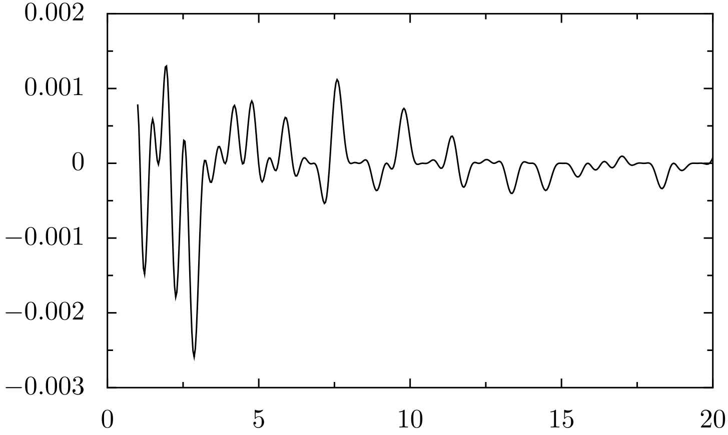
$$\int_0^\infty xJ_0(x\sqrt{2})J_0(x\sqrt{3})J_0(x\sqrt{5})J_0(x\sqrt{7})J_0(x\sqrt{11})dx,$$

where J_0 denotes the Bessel function of the first kind of order zero?

Integrand near 0



Integrand away from 0



Computational difficulties

- Infinite range
- Irregular oscillatory behaviour
- Slowly decaying integrand $\sim O(x^{-3/2})$

Possible solutions

- Extrapolation
- Double exponential formulas
- Integrate tail using incomplete Gamma function

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More general setting

Compute the value of

$$I(\boldsymbol{a}, \boldsymbol{\nu}, m) = \int_0^\infty x^m \prod_{i=1}^{k} J_{\nu_i}(a_i x) dx$$

where

- $J_{\nu_i}(x)$ Bessel function of the first kind and order ν_i
- m real number such that $\sum_i \nu_i + m > -1$ (assures integrable singularity at 0)
- a_i strictly positive real numbers

Applications

Integrals of this kind occur in ...

- Calculation of products of nucleon propagators in a spherically symmetric medium
- Evaluation of water melon type Feynman diagrams
- Particle motion in an unbounded rotating fluid in magnetohydrodynamic flow
- Crack problems in elasticity
- Distortions of nearly circular lipid domains
- ...

Algorithm — basic idea

Split integral in finite and infinite part at breakpoint x_0

Finite part

$$I_1 = \int_0^{x_0} x^m \prod_{i=1}^{k} J_{\nu_i}(a_i x) dx$$

- low-order composite Gauss-Legendre
- extrapolation to 0 if algebraic singularity

Infinite part

$$I_2 = \int_{x_0}^{\infty} x^m \prod_{i=1}^{k} J_{\nu_i}(a_i x) dx$$

- asymptotic expansion for J_{ν_i}
- integrate using incomplete Gamma function

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Finite part

- Split $[0, x_0]$ at equidistant points
- Number of subintervals $\sim$ estimated number of zeros in integrand using low-order approximation

$$J_\nu(x) \approx \sqrt{\frac{2}{\pi x}} \cos\left(x - \left(\frac{\nu}{2} + \frac{1}{4}\right)\pi\right).$$

- Hard-coded Gauss-Legendre rules on each subinterval until requested precision
- Average degree of quadrature rule to reach machine precision $\approx 15 + 19$ (error estimate included)

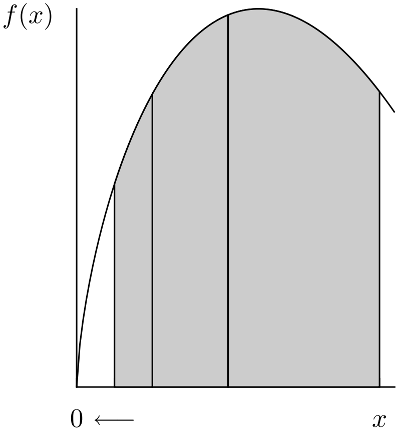
Finite part — extrapolation

Integrand $f(x)$ satisfies

$$f(x) = x^p \sum_{i=0}^{\infty} \alpha_i x^i, \quad x \to 0,$$

where $p = \sum_i \nu_i + m$.

- For non-integer p algebraic singularity in 0
- Extrapolate à la Richardson to remove singularity



Infinite part

There exist functions $P(\nu, x)$ and $Q(\nu, x)$ such that

$$J_\nu(x) = \sqrt{\frac{2}{\pi x}} \left[P(\nu, x) \cos \chi - Q(\nu, x) \sin \chi \right]$$

where $\chi = x - (\nu/2 + 1/4)\pi$.
P and Q admit known asymptotic expansions

$$P(\nu, x) \sim \sum_{j=0}^{\infty} c_{\nu,j} x^{-2j}$$

$$Q(\nu, x) \sim \sum_{j=0}^{\infty} d_{\nu,j} x^{-2j-1} \qquad x \longrightarrow \infty$$

Upper incomplete Gamma function

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

- Generalization of Gamma function $\Gamma(a) = \Gamma(a,0)$
- Extended to arbitrary complex a and x by analytic continuation
- Efficient evaluation using Legendre's continued fraction expansion

$$\Gamma(a,x) = \frac{e^{-x}x^a}{x+} \frac{1-a}{1+} \frac{1}{x+} \frac{2-a}{1+} \frac{2}{x+} \cdots$$

- From the definition we obtain

$$\int_{x_0}^\infty e^{\mathbf{i}\alpha x} x^\beta dx = \left(\frac{\mathbf{i}}{\alpha}\right)^{\beta+1} \Gamma(\beta+1, -\mathbf{i}\alpha x_0)$$

Evaluating infinite range integrals using $\Gamma(a, x)$

Starting from asymptotic expansion for J_ν ...

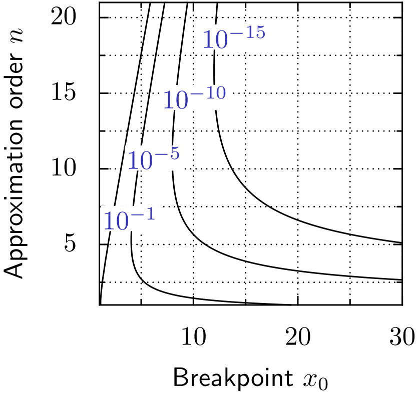
- Convert sine and cosine to exponentials
- Take $n+1$ terms in expansion
- Approximate tail of integrand

...leads to $2^{k-1}(k(2n+1)+1)$ integrals of the form

$$\int_{x_0}^{\infty} e^{\mathbf{i}\eta_i x} x^{m-k/2-j} dx, \quad i = 1, 2, \ldots, 2^{k-1}, \quad j = 0, 1, \ldots, k(2n+1)$$

where $\eta_i = a_1 \pm a_2 \pm \ldots \pm a_k$ (summing over all possible combinations).

Determining breakpoint x_0 and approximation order n



Contour plot of relative accuracy for infinite part $\delta(x_0, n)$

- *A priori* error estimates $\delta(x_0, n)$ and $\Delta(x_0, n)$ follow from error analysis
- Different (x_0, n) combinations lead to same accuracy
- Choose parameters to minimize computational effort

  $\rightarrow$ cost function

A suitable cost function

Major computational effort from evaluating Γ and J_ν

- On average $N = 15 + 19$ Bessel function evaluations in quadrature formula *per subinterval*
- Estimate number of subintervals from approximate number of zeros in integrand
- Incomplete Gamma function is called $2^{k-1}(k(2n+1)+1)$ times (at most)

Ignoring fixed cost gives cost function

$$\chi(x_0, n) = 2^k n t_{GJ} + \frac{x_0}{\pi} \frac{N}{2} \sum_{j=1}^{k} a_j$$

where t_{GJ} is relative efficiency of Γ compared to J_ν

Optimization problem

If relative error should not exceed ϵ

Find the values of x_0 and n which minize the cost function $\chi(x_0, n)$ with the constraint that $\delta(x_0, n) \leq \epsilon$

Using Lagrange multipliers leads to system of two nonlinear equations

$$\frac{\partial \delta}{\partial x_0} 2^k t_{GJ} = \frac{\partial \delta}{\partial n} \frac{N}{2\pi} \sum_{j=1}^{k} a_j \qquad (1)$$

$$\delta(x_0, n) = \epsilon$$

Approximate solution to (1) yields linear relation between x_0 and n

Nonlinear equation

Approximate optimal parameters (x_0, n) satisfy

$$x_0 = \frac{\kappa}{W(\kappa)} \left[n + \frac{1}{4} \left(3 - \frac{1}{1 + W(\kappa)} \right) \right]$$

where

$$\kappa = \frac{2^{k+1} t_{GJ} \pi}{N \sum_{j=1}^{k} a_j}.$$

and $W(x)$ is the Lambert W-function, $x = We^W$
Substituting in

$$\delta(x_0, n) = \epsilon$$

gives nonlinear equation in $n \rightarrow$ solve using Dekker-Brent

Matlab-programs

`igamma.m`

- Incomplete Gamma function
- Matlab's `gammainc.m` does not support complex arguments
- Fortran-to-Matlab conversion of program by Kostlan and Gokhman (1987)
- Small improvements

`besselint.m`

- Implementation of our algorithm
- Toolbox-independent
- Easy translation into other languages

Determining t_{GJ}

Definition

$$t_{GJ} = \frac{t_\Gamma}{t_J}$$

where

t_Γ average execution time for one call to `igamma`

t_J average execution time for one call to `besselj`

Problems

- Matlab supports vector operations $\longrightarrow$ average call to `besselj` has argument of size ≈ 17
- Cost function is not exact

gettGJ.m

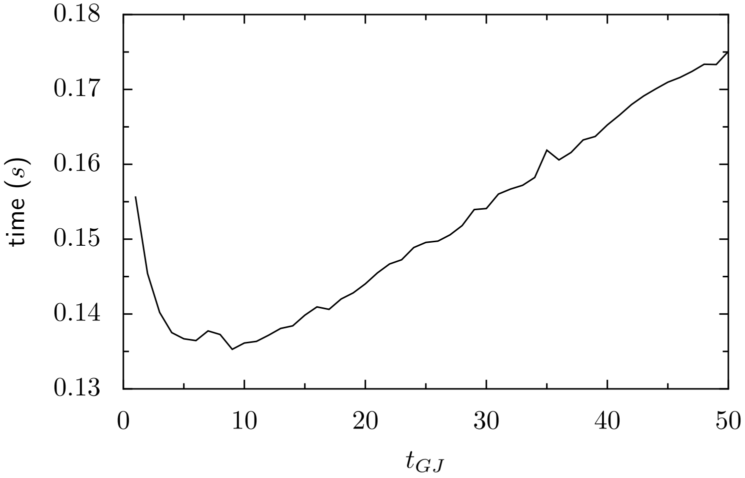
Implementation

- $2040 = 17 * 120$ calls to `igamma` (scalar argument) and `besselj` (vector argument)
- Partial loop unrolling to avoid zero timings on fast machines
- Averaging over 22 runs

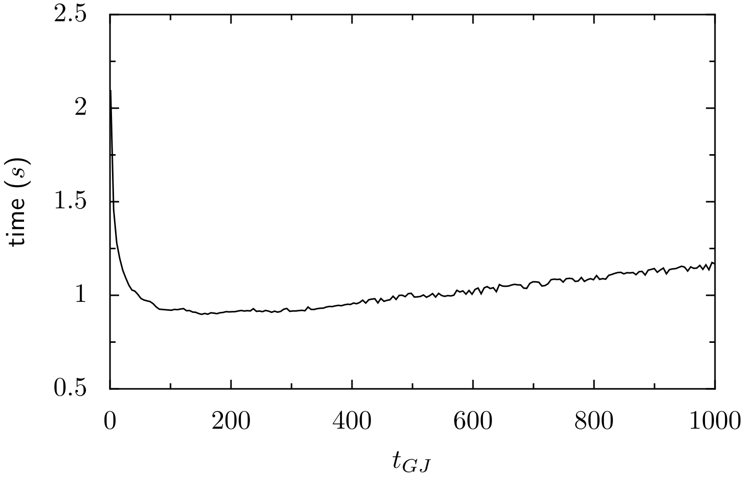
Results on Intel processor $2.80GHz$

	Matlab	Octave
t_{GJ}	19	1357

Execution time `besselint.m` vs. t_{GJ} — Matlab



Execution time `besselint.m` vs. t_{GJ} — Octave



Backward compatibility

Our code has been tested under

- Matlab 7.0.1.24704 (R14) Service Pack 1 for Linux,
- Matlab 6.5.0.180913a (R13) for Linux and Windows
- Matlab 6.1.0.450 (R12.1) for Windows
- Octave 2.1.69

Backward compatibility issues have negative impact on efficiency

Logical operators

Matlab ≥6.5 and Octave

	Short-circuit	Element-wise
and	&&	&
or	||	|

Matlab <6.5

- Only & and |
- Automatic short-circuit in condition after if-statement

Problem

- Because of backward compatibility we use & and |
- Makes `igamma` two times slower in Matlab 7.0

Numerical examples

Syntax for `besselint`

```
[f,err] = besselint(a,nu,m,reltol,abstol)
```

where

- `f` result
- `err` (optional) absolute and relative error estimates
- `a` vector with coefficients a_j
- `nu` vector with orders ν_j
- `m` power of x
- `reltol` (optional) relative tolerance
- `abstol` (optional) absolute tolerance

Excerpt from `experiments.m` with added timings

```
Part I: explicitly known examples

Ex. 1.2: a=[1]; nu=[-1/4]; m=1/3;
Exact answer: 4.699242939646014e-01
f =
     4.699242939646101e-01
time =
     9.648300000000098e-02
```

```
Ex. 2.1: a=[1 5]; nu=[0 1]; m=0;
Exact answer: 1/5
f =
     2.000000000000000e-01
time =
     1.373540000000002e-01

Ex. 4.1: a=sqrt([2 3 5 7]); nu=0; m=1;
Exact answer: 1.104110282210471e-01
f =
     1.104110282210470e-01
time =
     2.150379999999998e-01
```

```
Part II: how reliable are the error estimates?

Ex. 7.1: a=sqrt([2 3 5]); nu=0; m=1
Requested relative precision: 1e-14
Estimated relative precision: 2.35e-15
Actual relative precision: 1.67e-15

Ex. 8.2: a=sqrt([2 3 5 7]); nu=0; m=1
Requested absolute precision: 1e-6
Estimated absolute precision: 8.04e-07
Actual absolute precision: 4.11e-09
```

```
Part III: some unusual cases

Ex. 9.1: a=[1 1]; nu=0;  m=1;
Exact answer: -Inf
Assuming a(1)-a(2)=0;
Warning: Possible discontinuous case;
 result and error estimate may be inaccurate
> In besselint at 106
f =
  -Inf
time =
     1.103760000000005e-01
```

```
Ex. 11.1: a=[1 10 1000]; nu=0; m=1;
Exact answer: 0
f =
   -8.655453817121351e-17
time =
     4.545179000000001e+00

Ex. 11.3: a=1; nu=100; m=0;
Exact answer: 1
f =
     9.999999999989873e-01
time =
     8.703063000000000e+00
```