# Maxima by Example:

# Ch.9: Bigfloats and Arbitrary Precision Quadrature \*

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<sup>\*</sup>This version uses Maxima 5.18.1. This is a live document. Check http://www.csulb.edu/~woollett/ for the latest version of these notes. Send comments and suggestions to woollett@charter.net

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This document is part of a series of notes titled "Maxima by Example" and is made available via the author's webpage http://www.csulb.edu/~woollett/to aid new users of the Maxima computer algebra system.

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Feedback from readers is the best way for this series of notes to become more helpful to new users of Maxima. *All* comments and suggestions for improvements will be appreciated and carefully considered.

#### LOADING FILES

The defaults allow you to use the brief version load(brmbrg) to load in the Maxima file brmbrg.lisp.

To load in your own file, such as qbromberg.mac (used in this chapter), using the brief version load(qbromberg), you either need to place qbromberg.mac in one of the folders Maxima searches by default, or else put a line like:

file\_search\_maxima : append(["c:/work3/###.{mac,mc}"],file\_search\_maxima )\$

in your personal startup file maxima-init.mac (see Ch. 1, Getting Started for more information about this).

Otherwise you need to provide a complete path in double quotes, as in load("c:/work3/qbromberg.mac"),

We always use the brief load version in our examples, which are generated using the XMaxima graphics interface on a Windows XP computer, and copied into a fancy verbatim environment in a latex file which uses the fancyvrb and color packages.

We use qdraw.mac for plots (see Ch.5), which uses draw2d defined in share/draw/draw.lisp.

Maxima.sourceforge.net. Maxima, a Computer Algebra System. Version 5.18.1
 (2009). http://maxima.sourceforge.net/

## 9.1 Introduction

This chapter is divided into two sections.

In the first section we discuss the use of **bfoat**, including examples which also involve **fpprec**, **bfloatp**, **bfallroots**, **fpprintprec**, **print**, and **printf**. The second section of Chapter 9 presents examples of the use of Maxima for arbitrary precision quadrature (numerical integration). (In Chapter 8, we gave numerous examples of numerical integration using the Quadpack functions such as **quad\_qags** as well as **romberg**. Those examples all accepted the default floating point precision of Maxima).

Chapter 10 covers both Fourier transform and Laplace transform type integrals. Chapter 11 presents tools for the use of fast Fourier transforms with examples of use.

Software files developed for Ch. 9 and available on the author's web page include:

```
    fdf.mac, 2. qbromberg.mac.
    quad_de.mac, 4. quad_ts.mac, 5. quad_gs.mac.
```

# 9.2 The Use of Bigfloat Numbers in Maxima

## 9.2.1 Bigfloat Numbers Using bfloat, fpprec, and fpprintprec

**bfloat(expr)** converts all numbers and functions of numbers in **expr** to bigfloat numbers. You can enter explicit bigfloat numbers using the notation **2.38b0**, or **2.38b7**, or **2.38b-4**, for example. **bfloatp(val)** returns **true** if **val** is a bigfloat number, otherwise **false** is returned.

The number of significant digits in the resulting bigfloat is specified by the parameter **fpprec**, whose default value is **16**. The setting of **fpprec** does not affect computations on ordinary floating point numbers.

The underlying Lisp code has two variables: 1. **\$fpprec**, which defines the Maxima variable **fpprec** (which determines the number of DECIMAL digits requested for arithmetic), and 2. **fpprec** which is related to the number of bits used for the fractional part of the bigfloat, and which can be accessed from Maxima using **?fpprec**. We can also use the **:lisp foobar** construct to look at a lisp variable **foobar** from "inside" the Lisp interpreter. You do not end with a semi-colon; you just press ENTER to get the response, and the input line number of the Maxima prompt does not advance.

```
(%i1) fpprec;

(%o1) 16

(%i2) ?fpprec;

(%o2) 56

(%i3) :lisp $fpprec

16

(%i3) :lisp fpprec

56
```

We discuss some effects of the fact that computer arithmetic is carried out with binary bit representation of decimal numbers in Sec. 9.2.5.

## **Controlling Printed Digits with fpprintprec**

When using bigfloat numbers, the screen can quickly fill up with numbers with many digits, and **fpprintprec** allows you to control how many digits are displayed. For bigfloat numbers, when **fpprintprec** has a value between **2** and **fpprec** (inclusive), the number of digits printed is equal to **fpprintprec**. Otherwise, **fpprintprec** can be **0**, or greater than **fpprec**, in which case the number of digits printed is equal to **fpprec**. **fpprintprec** cannot be **1**. The setting of **fpprintprec** does not affect the precision of the bigfloat arithmetic carried out, only the setting of **fpprec** matters.

The parameter **fpprec** can be used as a local variable in a function defined using **block**, and set to a local value which does not affect the global setting. Such a locally defined value of **fpprec** governs the bigfloat calculations in that function and in any functions called by that function, and in any third layer functions called by the secondary layer functions, etc. **fpprintprec** can be set to a value inside a function defined with **block**, without changing the global value, provided you include the name **fpprintprec** in the local variables bracket [ ]:

```
(%i1) [fpprec, fpprintprec];
(%01)
                                      [16, 0]
(%i2) piby2 : block([fpprintprec,fpprec:30,val],
                  val:bfloat(%pi/2),
                  fpprintprec:8,
                  disp(val),
                   print(" ", val),
                   val);
                                    1.5707963b0
  1.5707963b0
                        1.57079632679489661923132169164b0
(%o2)
(%i3) [fpprec, fpprintprec];
(%o3)
                                      [16, 0]
```

For simple **bfloat** uses in interactive mode, one can use the syntax **bfloat-job**, **fpprec:fp**; which implicitly uses the **ev(...)** construct with temporary settings of global flags as in

```
(%i1) bfloat(%pi), fpprec:20;
                             3.1415926535897932385b0
(%o1)
(%i2) slength(string(%));
(%o2)
                                        23
(%i3) fpprec;
                                        16
(%o3)
(%i4) bfloat(%pi),fpprec:40;
(%04)
                   3.141592653589793238462643383279502884197b0
(%i5) slength(string(%));
(%05)
                                        43
(%i6) fpprec;
(%06)
(%i7) tval : bfloat(integrate(exp(x),x,-1,1)),fpprec:30;
(%07)
                        2.35040238728760291376476370119b0
(%i8) slength(string(%));
(%08)
                                        33
```

Next we illustrate passing both a bigfloat number as well as local values of **fpprec** and **fpprintprec** to a second function. Function **f1** is designed to call function **f2**:

And here we call f1 with values x = 0.5, fp = 30, fprt = 8:

We see that the called function (**f2**) maintains the values of **fpprec** and **fpprintprec** which exist in the calling function (**f1**).

Bigfloat numbers are "contagious" in the sense that, for example, multiplying (or adding) an integer or ordinary float number with a bigfloat results in a bigfloat number. In the above example sin(w) is a bigfloat since w is one.

```
(%i5) 1 + 2.0b0;

(%o5) 3.0b0

(%i6) 1.0 + 2.0b0;

(%o6) 3.0b0

(%i7) sin(0.5b0);

(%o7) 4.79425538604203b-1
```

The Maxima symbol %pi is not automatically converted by contagion (in the present version of Maxima), and an extra use of bfloat does the conversion.

A recent comment by Maxima developer Volker van Nek on the Maxima mailing list illustrates how the setting of **fpprec** can affect what is printed to the screen when doing bigfloat arithmetic.

Note that **1b-25** is the bigfloat version of  $10^{-25}$ . In the case above the value of **fpprec** is large enough to see the effect of the bigfloat addition. The number of digits identified by the conversion of the number to a string and then finding the length of the string is 29 - 3 = 26 since the three string characters [., b, 0] do not contribute to the precision of the number. If we leave the **fpprec** at **26** and add to **1** the bigfloat equivalent of  $10^{-26}$ , Maxima prints out a bigfloat version of **1**, but if we subtract from that answer **1b0** we do not get zero:

Of the thirty one characters present in this string, the five characters [., b, -, 2, 7] do not contribute to the precision, , leaving **26** digits of precision. Note that the setting of **fpprintprec** was **0** in the above, which provides for printing of the same number of significant digits as the value of **fpprec**.

Here are three ways to enter the bigfloat equivalent of  $1/10 = 10^{-1} = 0.1$ :

```
(%i18) [1b-1,bfloat(10^(-1)),10b0^(-1)];
(%o18) [1.0b-1, 1.0b-1, 1.0b-1]
```

We next show that once bigfloat numbers are in play inside a **block** function in which a local value of **fpprec** is set, the subsequent arithmetic is the same whether or not you wrap each operation with **bfloat**.

```
(%i19) test1(h,j,fp):=
 block([fpprec:fp,u,a,x,w],
  u:bfloat(h*j),
  a:bfloat(exp(-u)),
  x:bfloat(exp(u-a)),
  w:bfloat(exp(-a)+x),
   [x,w])$
(%i20) test2(h,j,fp):=
 block([fpprec:fp,u,a,x,w],
  u:bfloat(h*j),
  a: exp(-u),
  x: exp(u-a)
  w: exp(-a)+x,
   [x,w])$
(%i21) [xt, wt]:test1(1/16, 9, 60)$
(\%i22) [x1,w1]:test1(1/16,9,40)$
(%i23) [x2, w2]:test2(1/16, 9, 40)$
```

In the above, we used the "completely **bfloat** wrapped" version test1(..) to define answers with **60** digit precision, and then used test1(..) and test2(..) to compute comparison answers at **40** digit precision. We see that there is no difference in precision between the answers returned by the two test versions (each using 40 digit precision).

We also see, from the output %08, that arith\_job, fpprec:60; using interactive mode produces the same answer (with bigfloats already in play) whether or not the "arithmetic\_job" is wrapped in bfloat. The numbers returned by both test versions are bigfloats, as indicated by the last two outputs.

## 9.2.2 Using print and printf with Bigfloats

In Sec. 9.2.1 we described the relations between the settings of **fpprec** and **fpprintprec**. Once you have generated a bigfloat with some precision, it is convenient to be able to control how many digits are displayed. We start with the use of **print**. If you start with the global default value of **16** for **fpprec** and the default value of **0** for **fpprintprec**, you can use a simple one line command for a low number of digits, as shown in the following. We first define a bigfloat **bf1** to have **fpprec** = **45** digits of precision:

We then use **print** with **fpprintprec** to get increasing numbers of digits on the screen:

```
(%i4) print(bf1), fpprintprec:12$
2.35040238728b0
(%i5) [fpprec, fpprintprec];
                                      [16, 0]
(%i6) print(bf1), fpprintprec:15$
2.3504023872876b0
(%i7) [fpprec, fpprintprec];
                                      [16, 0]
(%i8) print(bf1), fpprintprec:16$
2.35040238728760291376476370119120163031143596b0
(%i9) [fpprec, fpprintprec];
(%09)
                                      [16, 0]
(%i10) slength(string(%o8));
                                        48
(%010)
```

As you see above, when **fpprintprec** reaches the global value of **fpprec = 16 all 45** digits are printed. To control the number of printed digits, you need to locally set the value of **fpprec** as shown here:

```
(%i11) print(bf1),fpprec:20,fpprintprec:18$
2.35040238728760291b0
```

To use this construct in a **do** loop, wrap it in **ev(...)**:

```
(%i12) for j:14 thru 18 do ev(print(bf1),fpprec:j+2,fpprintprec:j)$
2.3504023872876b0
2.350402387287602b0
2.3504023872876029b0
2.35040238728760291b0
```

A more formal approach is to define a small function which we call **bfprint**:

```
(%i13) bfprint(bf,fpp):=
block([fpprec, fpprintprec],
    fpprec : fpp+2,
    fpprintprec:fpp,
    print(" number of digits = ",fpp),
    print(" ",bf) )$
```

with the behavior:

```
(%i14) bfprint(bf1,24)$
number of digits = 24
2.35040238728760291376476b0
```

### Using printf with bigfloats

We first show some interactive use of **printf** with bigfloats.

The format string is enclosed in double quotes, with "d used for an integer, "f used for a floating point number, a used for a Maxima string, "e used for exponential display of a floating point number, and "h used for a bigfloat number. You can include the newline instruction with "% anywhere and as many times as you wish. In the example above, we used the string formatting to display the bigfloat number bf, which required that bf be converting to a Maxima string using **string**. Because we did not include any spaces between the integer format instruction "d and the string format character a, we get 32.0... instead of 3 2.0....

```
(%i4) printf(true, " ~d~a", 3, string(bf))$
32.06115362243855782796594038016b-9
(%i5) printf(true, " ~d ~a", 3, string(bf))$
3 2.06115362243855782796594038016b-9
```

To get the output on successive lines we had to include the newline instruction ~ %. To control the number of significant figures displayed, we use **fpprintprec**:

```
(%i8) fpprintprec:8$
(%i9) printf(true," ~d ~a",3,string(bf))$
3 2.0611536b-9
```

Next let's show what we get if we use the other options:

```
(%i10) printf(true," ~d ~f",3,bf)$
3  0.000000020611536224385579
(%i11) printf(true," ~d ~e",3,bf)$
3  2.0611536224385579E-9
(%i12) printf(true," ~d ~h",3,bf)$
3  0.0000000020611536
```

## A Table of Bigfloats using block and printf

Here is an example of using **printf** with bigfloats inside a **block** to make a table.

```
(%i1) print_test(fp) :=
       block([fpprec, fpprintprec, val],
        fpprec : fp,
        fpprintprec: 8,
        display(fpprec),
        print(" k
                            value "),
        print(" "),
        for k thru 4 do
          ( val : bfloat(exp(k^2)),
           printf(true," ~d
                                   ~a ~%",k,string(val) )))$
(%i2) print_test(30)$
                                  fpprec = 30
 k
            value
 1
         2.7182818b0
 2
         5.459815b1
 3
         8.1030839b3
         8.8861105b6
```

Note the crucial use of the newline instruction \(^{\infty}\) to get the table output. Some general use examples of **printf** can be found in the Maxima manual and in the file

```
C:\Program Files\Maxima-5.17.1\share\maxima\5.17.1\share\
contrib\stringproc\rtestprintf.mac
```

We can use **printf** for the titles and empty lines with the alternative version. We first define an alternative function **print\_test2**:

```
(%i3) print_test2(fp) :=
    block([fpprec,fpprintprec,val],
    fpprec : fp,
    fpprintprec : 8,
    display(fpprec),
    printf(true,""% ~a ~a ~%"%",k,value),
    for k thru 4 do
    ( val : bfloat(exp(k^2)),
        printf(true," ~d ~a ~%",k,string(val) ) ))$
```

Here we try out the alternative function with fp = 30:

## 9.2.3 Adding Bigfloats Having Differing Precision

If **A** and **B** are bigfloats with different precisions, the precision of the sum (**A** + **B**) is the precision of the least precise number. As an example, we calculate an approximation to  $\pi$  using both 30 and 50 digit precision, and add the numbers using 40 digit precision, and then using 60 digit precision. In both cases, the result has 30 digit precision.

```
(%i1) fpprintprec:8$
(%i2) pi50 : bfloat(%pi),fpprec:50;
(%o2)
                                    3.1415926b0
(%i3) pi30 : bfloat(%pi), fpprec:30;
                                    3.1415926b0
(%o3)
(%i4) abs(pi30 - pi50), fpprec:60;
(%04)
                                   1.6956855b-31
(%i5) twopi : bfloat(2*%pi), fpprec:60;
(%05)
                                    6.2831853b0
(%i6) pisum40 : pi30 + pi50, fpprec:40;
(%06)
                                    6.2831853b0
(%i7) abs(pisum40 - twopi), fpprec:60;
(%07)
                                   1.6956855b-31
(%i8) pisum60 : pi30 + pi50, fpprec:60;
                                    6.2831853b0
(%i9) abs(pisum60 - twopi),fpprec:60;
(%09)
                                   1.6956855b-31
```

## 9.2.4 Polynomial Roots Using bfallroots

The Maxima function **bfallroots** has the same syntax as **allroots**, and computes numerical approximations of the real and complex roots of a polynomial or polynomial equation of one variable. In all respects, **bfallroots** is identical to **allroots** except that **bfallroots** computes the roots using bigfloats. The source code of **bfallroots** with some comments is in the file **cpoly.lisp** in the **src** directory.

Our example is a cubic equation

$$x^3 + 3x^2 - 13x - 38 = 0 (9.1)$$

```
(%i1) (ratprint:false, fpprintprec:8)$
(%i2) e : x^3+3*x^2-13*x-38$
```

Let **r** be the list of symbolic roots returned by **solve**. Then **first** (**r**) will be the first symbolic root. For brevity, we only show this first sybolic root.

Now let **rf16** be the default floating point numerical value of the symbolic roots returned by **solve**, in which we use **rectform(float(r))**.

```
(%i5) rf16 : rectform(float(r));
(%o5) [- 4.4408921E-16 %i - 2.8051181, - 3.7793103, 3.5844283]
```

We see that due to floating point arithmetic errors, the first root in the returned list has a very small imaginary part. We will find that there are only real roots by using **allroots**:

```
(%i6) rar16 : map('rhs,allroots(e));
(%o6) [3.5844283, - 2.8051181, - 3.7793103]
```

Now let's compare with **bfallroots** using the default **fpprec** = **16**.

```
(%i7) rbf16: map('rhs,bfallroots(e));

(%o7) [3.5844283b0, - 2.805118b0, - 3.7793102b0]

(%i8) rbf16 - rar16;

(%o8) [0.0b0, 1.3322676b-15, - 1.2767564b-15]
```

We see small differences which are of the order of the default **16** digit precision being used.

Next, we use **bfallroots** with **fpprec** = 30 and compare the results.

```
(%i9) rbf30 : map('rhs,bfallroots(e)),fpprec:30;

(%o9) [3.5844283b0, - 2.805118b0, - 3.7793102b0]

(%i10) rbf30 - rbf16,fpprec:30;

(%o10) [9.2452682b-18, - 7.0517343b-17, 5.7609241b-18]
```

Instead of using bigfloats via **bfallroots**, we can use bigfloats by using **bfloat** directly on the exact symbolic roots **r** returned by **solve**.

We see that the differences are of the order of the 30 digit precision being used.

The conventional wisdom on the Maxima mailing list is that more accurate results are found if the expression **e** is multiplied by **%i**, as in **bfallroots**(**%i\*e**). We will test that advice here by using **%i\*e** with **30** digit precision, and also with **40** digit precision (in order to have a "true value" to use for comparisons).

```
(%i16) rbf30i : map('rhs,bfallroots(%i*e)),fpprec:30;
(%o16) [3.5844283b0 - 1.3363823b-51 %i, 1.0114221b-50 %i - 2.805118b0,
                                              - 8.7778395b-51 %i - 3.7793102b0]
(%i17) rbf30i : realpart(rbf30i);
                  [3.5844283b0, -2.805118b0, -3.7793102b0]
(%o17)
(%i18) rbf30i - rbf30, fpprec:30;
                    [0.0b0, 7.888609b-31, -1.5777218b-30]
(%o18)
(%i19) rbf40i : map('rhs,bfallroots(%i*e)),fpprec:40;
(\$o19) [3.5844283b0 - 2.687686b-55 %i, 2.0315714b-54 %i - 2.805118b0,
                                              - 1.7628028b-54 %i - 3.7793102b0]
(%i20) rbf40i : realpart(rbf40i);
(%o20)
                  [3.5844283b0, -2.805118b0, -3.7793102b0]
(%i21) rbf30 - rbf40i, fpprec:40;
(%o21)
              [- 2.2105568b-32, - 1.7332203b-30, 2.5441868b-30]
(%i22) rbf30i - rbf40i, fpprec:40;
(%o22)
               [-2.2105568b-32, -9.4435949b-31, 9.6646505b-31]
```

We see that two out of three of the **30** digit precision roots found using the %i\*e method are slightly more accurate.

## 9.2.5 Bigfloat Number Gaps and Binary Arithmetic

**fpprec** as set by the user is the number of DECIMAL digits being requested. In fact, the actual arithmetic is carried out with binary arithmetic. Due to the inevitably finite number of binary bits used to represent a floating point number there will be a range of floating point numbers which are not recognised as different.

For a simple example, let's take the case **fpprec = 4**. Consider the gap around the number x:bfloat(2/3) whose magnitude is less than 1. We will find that **?fpprec** has the value 16 and that Maxima behaves as if (for this case) the fractional part of a bigfloat number is represented by the state of a system consisting of 18 binary bits.

Let  $u = 2^{-18}$ . If we let x1 = x + u we get a number which is treated as having a nonzero difference from x. However, if we let w be a number which is one significant digit less than u, and define x2 = x + w, x2 is treated as having **zero** difference from x. Thus the gap in bigfloats around our chosen x is  $ulp = 2 \cdot 2^{-18} = 2^{-17}$ , and this gap should be the same size (as long as **fpprec = 4**) for any bigfloat with a magnitude less than 1.

If we consider a bigfloat number whose decimal magnitude is less than 1, its value is represented by a "fractional binary number". For the case that this fractional binary number is the state of 18 (binary) bits, the smallest base 2 number which can occur is the state in which all bits are off (0) except the least significant bit which is on (1), and the decimal equivalent of this fractional binary number is precisely  $2^{-18}$ . Adding two bigfloats (each of which has a decimal magnitude less than 1) when each is represented by the state of an 18 binary bit system (interpreted as a fractional binary number), it is not possible to increase the value of any one bigfloat by less than this smallest base 2 number.

```
(%i1) fpprec:4$
(%i2) ?fpprec;
(%o2)
                                         16
(%i3) x :bfloat(2/3);
                                      6.667b-1
(%o3)
(%i4) u : bfloat(2^(-18));
                                      3.815b-6
(%04)
(\%i5) x1 : x + u;
                                      6.667b-1
(%05)
(%i6) x1 - x;
(%06)
                                      1.526b-5
(\%i7) x2 : x + 3.814b-6;
(%07)
                                      6.667b-1
(\%i8) x2 - x;
                                        0.0b0
(%08)
(%i9) ulp : bfloat(2^(-17));
(%09)
                                      7.629b-6
```

In computer science Unit in the Last Place, or Unit of Least Precision, ulp(x), associated with a floating point number x is the gap between the two floating-point numbers closest to the value x. We assume here that the magnitude of x is less than 1. These two closest numbers will be x + u and x - u where u is the smallest positive floating point number which can be accurately represented by the systems of binary bits whose states are used to represent the fractional parts of the floating point numbers.

The amount of error in the evaluation of a floating-point operation is often expressed in ULP. We see that for **fpprec = 4**, 1 ULP is about  $8 \cdot 10^{-6}$ . An average error of 1 ULP is often seen as a tolerable error.

We can repeat this example for the case fpprec = 16.

```
(%i10) fpprec:16$
(%ill) ?fpprec;
(%o11)
                                        56
(%i12) x :bfloat(2/3);
                              6.666666666667b-1
(%o12)
(%i13) u : bfloat(2^(-58));
                              3.469446951953614b-18
(%o13)
(%i14) x1 : x + u;
                              6.666666666667b-1
(%o14)
(\%i15) x1 - x;
                              1.387778780781446b-17
(%o15)
(\%i16) \times 2 : x + 3.469446951953613b-18;
                              6.666666666667b-1
(%016)
(%i17) x2 - x;
                                       0.0b0
(%017)
(%i18) ulp : bfloat(2^(-57));
                              6.938893903907228b-18
(%o18)
```

## 9.2.6 Effect of Floating Point Precision on Function Evaluation

Increasing the value of **fpprec** allows a more accurate numerical value to be found for the value of a function at some point. A simple function which allows one to find the absolute value of the change produced by increasing the value of **fpprec** has been presented by Richard Fateman.\* This function is **uncert(f, arglist)**, in which **f** is a Maxima function, depending on one or more variables, and **arglist** is the n-dimensional point at which one wants the change in value of **f** produced by an increase of **fpprec** by **10**. This function returns a two element list consisting of the numerical value of the function at the requested point and also the absolute value of the difference induced by increasing the value of the current **fpprec** setting by the amount **10**.

We present here a version of Fateman's function which has an additional argument to control the amount of the increase of **fpprec**, and also has been simplified to accept only a function of one variable.

The function **fdf** is available in the Ch. 8 files **fdf.mac**, **qbromberg.mac**, **quad\_ts.mac**, and **quad\_de.mac**, and is defined by the code

```
fdf (%ff, %xx, %dfp) :=
  block([fv1,fv2,df],
  fv1:bfloat(%ff(bfloat(%xx))),
  block([fpprec:fpprec + %dfp ],
  fv2: bfloat(%ff(bfloat(%xx))),
  df: abs(fv2 - fv1) ),
  [bfloat(fv2),bfloat(df)] )$
```

Here is an example of how this function can be used.

```
(%i1) (fpprintprec:8,load(fdf))$
(%i2) fpprec;
(%o2) 16
(%i3) g(x) := sin(x/2)$
```

<sup>\*</sup>see his draft paper "Numerical Quadrature in a Symbolic/Numerical Setting", Oct. 16, 2008, available as the file **quad.pdf** in the folder: http://www.cs.berkeley.edu/~fateman/papers/

```
(%i4) fdf(g,1,10);

(%o4) [4.7942553b-1, 1.834924b-18]

(%i5) fdf(g,1,10),fpprec:30;

(%o5) [4.7942553b-1, 2.6824592b-33]

(%i6) fpprec;

(%o6) 16
```

In the first example, **fpprec** is **16**, and increasing the value to **26** produces a change in the function value of about  $2 \times 10^{-18}$ . In the second example, **fpprec** is **30**, and increasing the value to **40** produces a change in the function value of about  $3 \times 10^{-33}$ .

In the later section describing the "tanh-sinh" quadrature method, we will use this function for a heuristic estimate of the contribution of floating point errors to the approximate numerical value produced for an integral by that method.

## 9.3 Arbitrary Precision Quadrature with Maxima

## 9.3.1 Using bromberg for Arbitrary Precision Quadrature

A bigfloat version of the **romberg** function is defined in the file **brmbrg.lisp** located in **share/numeric**. You need to use **load(brmbrg)** or **load("brmbrg.lisp")** to use the function **bromberg**.

The use of **bromberg** is identical to the use of the **romberg** which we discussed in Chapter 8 (Numerical Integration), except that **rombergtol** (used for a relative error precision return) is replaced by the bigfloat **brombergtol** with a default value of **1.0b-4**, and **rombergabs** (used for an absolute error return) is replaced by the bigfloat **brombergabs** which has the default value **0.0b0**, and **rombergit** (which causes an return after halving the step size that many times) is replaced by the integer **brombergit** which has the default value **11**, and finally, **rombergmin** (the minimum number of halving iterations) is replaced by the integer **brombergmin** which has the default value **0**.

If the function being integrated has a magnitude of order one over the domain of integration, then an absolute error precision of a given size is approximately equivalent to a relative error precision of the same size. We will test **bromberg** using the function **exp(x)** over the domain [-1, 1], and use only the absolute error precision parameter **brombergabs**, setting **brombergtol** to **0.0b0** so that the relative error test cannot be satisfied. Then the approximate value of the integral is returned when the absolute value of the change in value from one halving iteration to the next is less than the bigfloat number **brombergabs**.

We explore the use and behavior of **bromberg** for the simple integral  $\int_{-1}^{1} e^{x} dx$ , binding a value accurate to 42 digits to **tval**, defining parameter values, calling **bromberg** first with **fpprec** equal to 30 together with **brombergabs** set to **1.0b-15** and find an actual error (compared with **tval**) of about  $7 \times 10^{-24}$ .

We see that, for the case of this test integral involving a well behaved integrand, the actual error of the result returned by **bromberg** is much smaller than the requested "difference error" supplied by the parameter **brombergabs**.

For later use, we define **qbromberg** (in a file **qbromberg.mac**) with the code:

This function, with the syntax

```
qbromberg ( f, a, b, rprec, fp, itmax )
```

uses the Maxima function **bromberg** to integrate the Maxima function  $\mathbf{f}$  over the interval  $[\mathbf{a}, \mathbf{b}]$ , setting the local value of **fpprec** to  $\mathbf{fp}$ , setting **brombergtol** to  $\mathbf{0}$ , setting **brombergabs** to  $\mathbf{10}^{-\text{rprec}}$ , where **rprec** is called the "requested precision".

Here is a test of **qbromberg** for this simple integral.

We have to be careful in the above step by step method to set **fpprec** to a large enough value to see the actual size of the error in the returned answer.

Instead of the work involved in the above step by step method, it is more convenient to define a function **qbrlist** which is passed a desired **fpprec** as well as a list of requested precision goals for **bromberg**. The function **qbrlist** then assumes a sufficiently accurate **tval** is globally defined, and proceeds through the list to calculate the **bromberg** value for each requested precision, computes the error in the result, and prints a line containing (rprec, fpprec, value, value-error). Here is the code for such a function, available in **qbromberg.mac**:

```
qbrlist(%f,a,b,rplist,fp,itmax) :=
  block([fpprec:fp,fpprintprec,brombergtol,
             brombergabs, brombergit, val, verr, pr],
     if not listp(rplist) then (print("rplist # list"), return(done)),
     brombergtol: 0.0b0,
     brombergit : itmax,
     fpprintprec:8,
                                                  verr "),
     print(" rprec
                      fpprec
                                 val
     print(" "),
     for pr in rplist do
      ( brombergabs : bfloat(10^(-pr)),
        val: bromberg(%f(x),x,a,b),
        verr: abs(val - tval),
        print(" ",pr,"
                           ",fp,"
                                    ", val, "
                                               ", verr) ) )$
```

and here is an example of use of **qbrlist** in which the requested precision **rprec** (called **pr** in the code) is set to three different values supplied by the list **rplist** for each setting of **fpprec** used. We first define an accurate comparison value **tval**:

Here is our test for three different values of **fpprec**:

```
(%i3) qbrlist(exp,-1,1,[10,15,17],20,100)$
rprec
         fpprec
                    val
                                    verr
                                  4.5259436b-14
  10
          20
                 2.3504023b0
  15
          20
                 2.3504023b0
                                 1.3552527b-20
  17
          20
                 2.3504023b0
                                 1.3552527b-20
(%i4) qbrlist(exp,-1,1,[10,20,27],30,100)$
rprec
         fpprec
                    val
                                    verr
  10
          30
                                 4.5259437b-14
                 2.3504023b0
  20
          30
                 2.3504023b0
                                 1.4988357b-29
  27
          30
                 2.3504023b0
                                 5.5220263b-30
(%i5) qbrlist(exp,-1,1,[10,20,30,35],40,100)$
rprec
         fpprec
                    val
                                    verr
  10
          40
                 2.3504023b0
                                 4.5259437b-14
  20
          40
                 2.3504023b0
                                 1.0693013b-29
  30
          40
                 2.3504023b0
                                 1.1938614b-39
  35
          40
                 2.3504023b0
                                  1.1938614b-39
```

We see that with **fpprec** equal to **40**, increasing **rprec** from **30** to **35** results in no improvement in the actual error of the result.

## When bromberg Fails

If the integrand has end point algebraic and/or logarithmic singularities, **bromberg** may fail. Here is an example in which the integrand has a logarithmic singularity at the lower end point:  $\int_0^1 \sqrt{t} \ln(t) dt$ . The **integrate** function has no problem with this integral.

You can instead use the tanh-sinh quadrature method for this integral (see Sec. 9.3.3).

## 9.3.2 A Double Exponential Quadrature Method for $a \le x < \infty$

This method (H. Takahasi and M. Mori, 1974; see Sec 9.3.3) is effective for integrands which contain a factor with some sort of exponential damping as the integration variable becomes large.

An integral of the form  $\int_{\mathbf{a}}^{\infty} \mathbf{g}(\mathbf{y}) \, d\mathbf{y}$  can be converted into the integral  $\int_{\mathbf{0}}^{\infty} \mathbf{f}(\mathbf{x}) \, d\mathbf{x}$  by making the change of variable of integration  $\mathbf{y} \to \mathbf{x}$  given by  $\mathbf{y} = \mathbf{x} + \mathbf{a}$ . Then  $\mathbf{f}(\mathbf{x}) = \mathbf{g}(\mathbf{x} + \mathbf{a})$ .

The double exponential method used here then converts the integral  $\int_0^\infty f(x) dx$  into the integral  $\int_{-\infty}^\infty F(u) du$  using a variable transformation  $x \to u$ :

$$\mathbf{x}(\mathbf{u}) = \exp(\mathbf{u} - \exp(-\mathbf{u})) \tag{9.2}$$

and hence

$$\mathbf{F}(\mathbf{u}) = \mathbf{f}(\mathbf{x}(\mathbf{u})) \, \mathbf{w}(\mathbf{u}), \qquad \text{where} \qquad \mathbf{w}(\mathbf{u}) = \frac{\mathbf{d}\mathbf{x}}{\mathbf{d}\mathbf{u}} = \exp(-\exp(-\mathbf{u})) + \mathbf{x}(\mathbf{u}). \tag{9.3}$$

You can confirm that  $\mathbf{x}(0) = \exp(-1)$ ,  $\mathbf{w}(0) = 2\mathbf{x}(0)$  and that  $\mathbf{x}(-\infty) = 0$ ,  $\mathbf{x}(\infty) = \infty$ .

Because of the rapid decay of the integrand when the magnitude of  $\mathbf{u}$  is large, one can approximate the value of the infinite domain  $\mathbf{u}$  integral by using a trapezoidal numerical approximation with step size  $\mathbf{h}$  using a modest number  $(2\,N+1)$  of function evaluations.

$$I(h, N) \simeq h \sum_{j=-N}^{N} F(u_j)$$
 where  $u_j = j h$  (9.4)

This method is implemented in the Ch. 8 file **quad\_de.mac**. We first demonstrate the available functions on the simple integral  $\int_0^\infty e^{-x} dx = 1$ .

```
(%i4) load(quad_de);

(%o4) c:/work3/quad_de.mac

(%i5) quad_de(g,0,30,40);

(%o5) [1.0b0, 4, 4.8194669b-33]

(%i6) abs(first(%) - tval),fpprec:45;

(%o6) 9.1835496b-41
```

The package function  $\mathbf{quad\_de}(\mathbf{f}, \mathbf{a}, \mathbf{rp}, \mathbf{fp})$  integrates the Maxima function  $\mathbf{f}$  over the domain  $[\mathbf{a}, \infty]$ , using  $\mathbf{fpprec}: \mathbf{fp}$ , and returns a three element list when  $\mathbf{vdiff}$  (the absolute value of the difference obtained for the integral in successive k levels) becomes less than or equal to  $\mathbf{10^{-rp}}$ . The parameter  $\mathbf{rp}$  is called the "requested precision", and the value of  $\mathbf{h}$  is repeatedly halved until the  $\mathbf{vdiff}$  magnitude either satisfies this criterion or starts increasing. The first element is the appoximate value of the integral. The second element (4 above) is the "final k level" used, where  $\mathbf{h} = \mathbf{2^{-k}}$ . The third and last element is the final value of  $\mathbf{vdiff}$ . We see in the above example that requesting precision  $\mathbf{rp} = \mathbf{30}$  and using floating point precision  $\mathbf{fpprec}: \mathbf{40}$  results in an answer good to about  $\mathbf{40}$  digits. This sort of accuracy is typical.

The package function idek(f, a, k, fp) integrates the Maxima function f over the domain  $[a, \infty]$  using a "k level approximation" with  $h = 1/2^k$  and fpprec: fp.

```
(%i7) idek(g,0,4,40);
(%o7) 1.0b0
(%i8) abs(% - tval),fpprec:45;
(%o8) 9.1835496b-41
```

The package function idek\_e(f, a, k, fp) does the same calculation as idek(f, a, k, fp), but returns both the approximate value of the integral and also a rough estimate of the amount of the error which is due to the floating point arithmetic precision being used. (The error of the approximation has three contributions: 1. the quadrature algorithm being used, 2. the step size h being used, and 3. the precision of the floating point arithmetic being used.)

```
(%i9) idek_e(g,0,4,40);
(%o9) [1.0b0, 8.3668155b-42]
(%i10) abs(first(%) - tval),fpprec:45;
(%o10) 9.1835496b-41
```

The package function ide(f, a, rp, fp) follows the same path as quad\_de(f, a, rp, fp), but shows the progression toward success as the k level increases (and h decreases):

```
(\%i11) ide(g, 0, 30, 40);
      rprec = 30 fpprec =
k
                        vdiff
       value
1
      1.0b0
2
      1.0b0
                      4.9349774b-8
3
      9.999999b-1
                     4.8428706b-16
4
      1.0b0
                      4.8194669b-33
```

The package function ide\_test(f, a, rp, fp) follows the path of ide(f, a, rp, fp), but adds to the table the value of the error of the approximate result for each k level attempted. The use of this function depends on an accurate value of the integral being bound to the global variable tval.

```
(%i12) ide_test(g,0,30,40);
     rprec = 30 fpprec =
k
      value
                       vdiff
                                        verr
1
     1.0b0
                                      4.9349775b-8
2
     1.0b0
                     4.9349774b-8
                                      4.8428706b-16
                                      4.8194668b-33
3
     9.999999b-1
                     4.8428706b-16
4
                     4.8194669b-33
     1.0b0
                                      9.1835496b-41
```

## **Test Integral 1**

Here we test this double exponential method code with the known integral

$$\int_0^\infty \frac{e^{-t}}{\sqrt{t}} dt = \sqrt{\pi}$$
 (9.5)

```
(\%i13) g(x) := exp(-x)/sqrt(x)$
(%i14) integrate(g(t),t,0,inf);
                                     sqrt(%pi)
(%o14)
(%i15) tval : bfloat(%),fpprec:45;
                                    1.7724538b0
(%o15)
(%i16) quad_de(g,0,30,40);
(%016)
                         [1.7724538b0, 4, 1.0443243b-34]
(%i17) abs(first(%) - tval), fpprec:45;
                                   1.8860005b-40
(%o17)
(%i18) idek_e(g, 0, 4, 40);
                          [1.7724538b0, 2.7054206b-41]
(%o18)
```

Again we see that the combination  $\mathbf{rp} = 30$ ,  $\mathbf{fp} = 40$  leads to an answer good to about 40 digits of precision.

## **Test Integral 2**

Our second known integral is

$$\int_0^\infty e^{-t^2/2} dt = \sqrt{\pi/2}$$
 (9.6)

## **Test Integral 3**

Our third test integral is

$$\int_0^\infty e^{-t} \cos t \, dt = 1/2 \tag{9.7}$$

## 9.3.3 The tanh-sinh Quadrature Method for $a \le x \le b$

H. Takahasi and M. Mori (1974: see references at the end of this section) presented an efficient method for the numerical integration of the integral of a function over a finite domain. This method is known under the names "tanh-sinh method" and "double exponential method". This method can handle integrands which have algebraic and logarithmic end point singularities, and is well suited for use with arbitrary precision work.

Quoting (loosely) David Bailey's (see references below) slide presentations on this subject:

The tanh-sinh quadrature method can accurately handle all "reasonable functions", even those with "blow-up singularities" or vertical slopes at the end points of the integration interval. In many cases, reducing the step size h by half doubles the number of correct digits in the result returned ("quadratic convergence").

An integral of the form  $\int_a^b g(y) \, dy$  can be converted into the integral  $\int_{-1}^1 f(x) \, dx$  by making the change of variable of integration  $y \to x$  given by  $y = \alpha x + \beta$  with  $\alpha = (b-a)/2$  and  $\beta = (a+b)/2$ . Then  $f(x) = \alpha g(\alpha x + \beta)$ .

The tanh-sinh method introduces a change of variables  $x \rightarrow u$  which implies

$$\int_{-1}^{1} \mathbf{f}(\mathbf{x}) \, d\mathbf{x} = \int_{-\infty}^{\infty} \mathbf{F}(\mathbf{u}) \, d\mathbf{u}. \tag{9.8}$$

The change of variables is expressed by

$$\mathbf{x}(\mathbf{u}) = \tanh\left(\frac{\pi}{2}\sinh\mathbf{u}\right) \tag{9.9}$$

and you can confirm that

$$u = 0 \Rightarrow x = 0, \qquad u \to -\infty \Rightarrow x \to -1, u \to \infty \Rightarrow x \to 1$$
 (9.10)

We also have  $\mathbf{x}(-\mathbf{u}) = -\mathbf{x}(\mathbf{u})$ .

The "weight"  $\mathbf{w}(\mathbf{u}) = \mathbf{dx}(\mathbf{u})/\mathbf{du}$  is

$$\mathbf{w}(\mathbf{u}) = \frac{\frac{\pi}{2} \cosh \mathbf{u}}{\cosh^2 \left(\frac{\pi}{2} \sinh \mathbf{u}\right)} \tag{9.11}$$

with the property  $\mathbf{w}(-\mathbf{u}) = \mathbf{w}(\mathbf{u})$ , in terms of which  $\mathbf{F}(\mathbf{u}) = \mathbf{f}(\mathbf{x}(\mathbf{u}) \, \mathbf{w}(\mathbf{u})$ . Moreover,  $\mathbf{F}(\mathbf{u})$  has "double exponential behavior" of the form

$$\mathbf{F}(\mathbf{u}) \approx \exp\left(-\frac{\pi}{2}\exp(\mid \mathbf{u}\mid)\right)$$
 for  $\mathbf{u} \to \pm \infty$ . (9.12)

Because of the rapid decay of the integrand when the magnitude of  $\mathbf{u}$  is large, one can approximate the value of the infinite domain integral by using a trapezoidal numerical approximation with step size  $\mathbf{h}$  using a modest number  $(2\,N+1)$  of function evaluations.

$$I(h, N) \simeq h \sum_{j=-N}^{N} F(u_j)$$
 where  $u_j = j h$  (9.13)

This method is implemented in the Ch.8 file **quad\_ts.mac** and we will illustrate the available functions using the simple integral  $\int_{-1}^{1} e^{x} dx$ .

The package function  $\mathtt{quad\_ts}$  (f, a, b, rp, fp) is the most useful workhorse for routine use, and uses the tanh-sinh method to integrate the Maxima function f over the finite interval [a, b], stopping when the absolute value of the difference  $(I_k - I_{k-1})$  is less than  $10^{-rp}$  (rp is the "requested precision" for the result), using fp digit precision arithmetic (fpprec set to fp, and bfloat being used to enforce this arithmetic precision). This function returns the list

[ approx-value, k-level-used, abs(vdiff) ], where the last element should be smaller than  $10^{-\mathrm{rp}}$  .

```
(%i1) fpprintprec:8$
(%i2) tval : bfloat(integrate(exp(x),x,-1,1)),fpprec:45;
                                  2.3504023b0
(%i3) load(quad ts);
   _kmax% = 8 _epsfac% = 2
                            c:/work3/quad ts.mac
(%i4) bfprint(tval, 45)$
  number of digits = 45
  2.35040238728760291376476370119120163031143596b0
(%i5) quad_ts(exp,-1,1,30,40);
construct _yw%[kk,fpprec] array for kk = 8 and fpprec = 40 ...working...
(%05)
                            [2.3504023b0, 5, 0.0b0]
(%i6) abs(first(%) - tval), fpprec:45;
                                 2.719612b-40
(%06)
```

A value of the integral accurate to about 45 digits is bound to the symbol **tval**. The package function **bfprint(bf, fpp)** allows controlled printing of **fpp** digits of the "true value" **tval** to the screen. We then compare the approximate quadrature result with this "true value". The package **quad\_ts.mac** defines two global parameters. **\_kmax**% is the maximum "k-level" possible (the defined default is 8, which means the minimum step size for the transformed "u-integral" is  $du = h = 1/2^8 = 1/256$ . The actual "k-level" needed to return a result with the requested precision **rp** is the integer in the second element of the returned list. The global parameter **\_epsfac**% (default value **2**) is used to decide how many **(y, w)** numbers to pre-compute (see below).

We see that a "k-level" approximation with k = 5 and  $h = 1/2^5 = 1/32$  returned an answer with an actual precision of about 40 digits (when rp = 30 and fp = 40).

The first time 40 digit precision arithmetic is called for, a set of (y, w) numbers are calculated and stored in an array which we call yw [8, 40]. The y(u) values will later be converted to x(u) numbers using high precision, and the original integrand function f(x(u)) is also calculated at high precision. The w(u) numbers are what we call "weights", and are needed for the numbers F(u) = f(x(u)) w(u) used in the trapezoidal rule evaluation. The package precomputes pairs (y, w) for larger and larger values of u until the magnitude of the weight w becomes less than eps, where  $eps = 10^{-np}$ , where  $eps = 10^{-np}$ , where  $eps = 10^{-np}$  is the global parameter epsfac% (default 2) and  $eps = 10^{-np}$  is the requested floating point precision  $eps = 10^{-np}$ .

Once the set of **40-digit** precision (y, w) numbers have been "pre-computed", they can be used for the evaluation of any similar precision integrals later, since these numbers are independent of the actual function being integrated, but depend only on the nature of the tanh-sinh transformation being used.

The package function qtsk(f, a, b, k, fp) (note: arg k replaces rp) integrates the Maxima function f over the domain [a, b] using a "k-level approximation" with  $h = 1/2^k$  and fpprec: fp.

```
(%i7) qtsk(exp,-1,1,5,40);
(%o7) 2.3504023b0
(%i8) abs(% - tval),fpprec:45;
(%o8) 2.719612b-40
```

A heuristic value of the error contribution due to the arithmetic precision being used (which is separate from the error contribution due to the nature of the algorithm and the step size being used) can be found by using the package function <code>qtsk\_e(f, a, b, k, fp)</code>;. The first element of the returned list is the value of the integral, the second element of the returned list is a rough estimate of the contribution of the floating point arithmetic precision being used to the error of the returned answer.

```
(%i9) qtsk_e(exp,-1,1,5,40);
(%o9) [2.3504023b0, 2.0614559b-94]
(%i10) abs(first(%) - tval),fpprec:45;
(%o10) 2.719612b-40
```

The very small estimate of the arithmetic precision contribution (two parts in  $10^{94}$ ) to the error of the answer is due to the high precision being used to convert from the pre-computed y to the needed abcissa x via x : bfloat(1-y) and the subsequent evaluation f(x). The precision being used depends on the size of the smallest y number, which will always be that appearing in the last element of the hashed array yw [8, 40].

```
(%i11) last(_yw%[8,40]);
(%o11) [4.7024891b-83, 8.9481574b-81]
```

(In Eq. (9.13) we have separated out the  $(\mathbf{u} = \mathbf{0}, \mathbf{x} = \mathbf{0})$  term, and used the symmetry properties  $\mathbf{x}(-\mathbf{u}) = -\mathbf{x}(\mathbf{u})$ , and  $\mathbf{w}(-\mathbf{u}) = \mathbf{w}(\mathbf{u})$  to write the remainder as a sum over positive values of  $\mathbf{u}$  (and hence positive values of  $\mathbf{x}$ ) so only the large  $\mathbf{u}$  values of  $\mathbf{y}(\mathbf{u})$  need to be pre-computed).

We see that the smallest y number is about  $5 \times 10^{-83}$  and if we subtract this from 1 we will get 1 unless we use a very high precision. It turns out that as u approaches plus infinity, x (as used here) approaches b (which is 1 in our example) from values less than b. Since a principal virtue of the tanh-sinh method is its ability to handle integrands which "blow up" at the limits of integration, we need to make sure we stay away (even if

only a little) from those end limits.

We can see the precision with which the arithmetic is being carried out in this crucial step by using the **fpxy(fp)** function

```
(%i12) fpxy(40)$
the last y value = 4.7024891b-83
the fpprec being used for x and f(x) is 93
```

and this explains the small number returned (as the second element) by qtsk\_e (exp, -1, 1, 5, 40);.

The package function qts(f, a, b, rp, fp) follows the same path as quad\_ts(f, a, b, rp, fp), but shows the progression toward success as the k level increases ( and h decreases ):

```
(\%i13) qts(exp,-1,1,30,40)$
 rprec = 30
                fpprec = 40
 k
          newval
                         vdiff
 1
      2.350282b0
      2.3504023b0
                      1.2031242b-4
 2
 3
      2.3504023b0
                      8.136103b-11
 4
       2.3504023b0
                      1.9907055b-23
 5
      2.3504023b0
                      0.0b0
```

The package function qts\_test(f, a, b, rp, fp) follows the path of qts(f, a, b, rp, fp), but adds to the table the value of the error of the approximate result for each k level attempted. The use of this function depends on an accurate value of the integral being bound to the global variable tval.

```
(%i14) qts_test(exp,-1,1,30,40)$
     rprec = 30 fpprec = 40
k
      value
                      vdiff
                                        verr
1
     2.350282b0
                                      1.2031234b-4
2
     2.3504023b0
                    1.2031242b-4
                                      8.136103b-11
3
     2.3504023b0
                    8.136103b-11
                                      1.9907055b-23
4
                    1.9907055b-23
                                      2.7550648b-40
     2.3504023b0
5
     2.3504023b0
                                      2.7550648b-40
                    0.0b0
```

#### **Test Integral 1**

Here we test this tanh-sinh method code with the known integral which confounded **bromberg** in Sec. 9.3.1:

$$\int_0^1 \sqrt{t} \ln(t) dt = -4/9 \tag{9.14}$$

Requesting thirty digit accuracy with forty digit arithmetic returns a value for this integral which has about forty digit precision. Note that "vdiff" is approximately the same as the actual absolute error.

## **Test Integral 2**

Consider the integral

$$\int_{0}^{1} \frac{\arctan(\sqrt{2+t^2})}{(1+t^2)\sqrt{2+t^2}} \, dt = 5 \, \pi^2/96. \tag{9.15}$$

```
(\%i20) g(x) := atan(sqrt(2+x^2))/(sqrt(2+x^2)*(1+x^2))$
(%i21) integrate(g(t),t,0,1);
                             atan(sqrt(t + 2))
(%o21)
                          / (t + 1) sqrt(t + 2)
(%i22) quad_qags(g(t),t,0,1);
                       [0.514042, 5.70701148E-15, 21, 0]
(%i23) float (5*%pi^2/96);
(%o23)
                                    0.514042
(%i24) tval: bfloat(5*%pi^2/96),fpprec:45;
                                 5.1404189b-1
(%o24)
(%i25) quad_ts(g,0,1,30,40);
                       [5.1404189b-1, 5, 1.5634993b-36]
(%o25)
(%i26) abs(first(%) - tval), fpprec:45;
                                 7.3300521b-41
(%o26)
(\%i27) qtsk_e(g,0,1,5,40);
                         [5.1404189b-1, 1.3887835b-43]
(%o27)
```

## **Test Integral 3**

We consider the integral

$$\int_{0}^{1} \frac{\sqrt{t}}{\sqrt{1-t^{2}}} dt = 2\sqrt{\pi} \Gamma(3/4)/\Gamma(1/4) \tag{9.16}$$

```
(\%i28) g(x) := sqrt(x)/sqrt(1 - x^2)$
(%i29) quad_qags(g(t),t,0,1);
                      [1.1981402, 8.67914629E-11, 567, 0]
(%o29)
(%i30) integrate(g(t),t,0,1);
                                        1 3
                                   beta(-, -)
(%o30)
(%i31) tval : bfloat(%),fpprec:45;
                                    1.1981402b0
(%o31)
(%i32) quad_ts(g,0,1,30,40);
                        [1.1981402b0, 5, 1.3775324b-40]
(%i33) abs(first(%) - tval), fpprec:45;
                                  1.8628161b-40
(%o33)
(\%i34) qtsk_e(g,0,1,5,40);
(%o34)
                         [1.1981402b0, 1.5833892b-45]
```

An alternative route to the "true value" is to convert **beta** to **gamma**'s using **makegamma**:

```
(%i35) makegamma(%o30);

2 sqrt(%pi) gamma(-)

4
(%o35)

1 gamma(-)

4
(%i36) float(%);
(%o36)

1.1981402
(%i37) bfloat(%o11), fpprec:45;
(%o37)

1.1981402b0
```

## **Test Integral 4**

We next consider the integral

$$\int_0^1 \ln^2 t \, dt = 2 \tag{9.17}$$

```
(%i38) g(x) := log(x)^2$
(%i39) integrate(g(t),t,0,1);
(%o39) 2
(%i40) quad_ts(g,0,1,30,40);
(%o40) [2.0b0, 5, 0.0b0]
(%i41) abs(first(%) - bfloat(2)),fpprec:45;
(%o41) 1.8367099b-40
(%i42) qtsk_e(g,0,1,5,40);
(%o42) [2.0b0, 1.2570464b-42]
```

## **Test Integral 5**

We finally consider the integral

$$\int_0^{\pi/2} \ln(\cos t) \, dt = -\pi \, \ln(2)/2 \tag{9.18}$$

```
(\%i46) float (-\%pi*log(2)/2);
(%046)
                                   -1.088793
(%i47) tval : bfloat(-%pi*log(2)/2),fpprec:45;
                                  -1.088793b0
(%047)
(%i48) quad_ts(g,0,%pi/2,30,40);
               [1.2979374b-80 \%i - 1.088793b0, 5, 9.1835496b-41]
(%048)
(%i49) ans: realpart(first(%));
                                   - 1.088793b0
(%049)
(%i50) abs(ans - tval), fpprec:45;
                                  1.9661653b-40
(%050)
(%i51) qtsk_e(g,0,%pi/2,5,40);
                [1.2979374b-80 \%i - 1.088793b0, 2.4128523b-42]
(%o51)
```

We see that the tanh-sinh result includes a tiny imaginary part due to bigfloat errors, and taking the real part produces an answer good to about 40 digits (using  $\mathbf{rp} = 30$ ,  $\mathbf{fp} = 40$ ).

## References for the tanh-sinh Quadrature Method

This method was initially described in the article **Double Exponential Formulas for Numerical Integration**, by Hidetosi Takahasi and Masatake Mori, in the journal Publications of the Research Institute for Mathematical Sciences (Publ. RIMS), vol.9, Number 3, (1974), 721-741, Kyoto University, Japan. A recent summary by the second author is **Discovery of the Double Exponential Transformation and Its Developments**, by Masatake Mori, Publ. RIMS, vol.41, Number 4, (2005), 897-935. Both of the above articles can be downloaded from the Project Euclid RIMS webpage

```
http://projecteuclid.org/
DPubS?service=UI&version=1.0&verb=Display&page=past&handle=euclid.prims
```

A good summary of implementation ideas can be found in the report **Tanh-Sinh High-Precision Quadrature**, by David H. Bailey, Jan. 2006, LBNL-60519, which can be downloaded from the webpage

```
http://crd.lbl.gov/~dhbailey/dhbpapers/
```

#### Further Improvements for the tanh-sinh Quadrature Method

The code provided in the file quad ts.mac has been lightly tested, and should be used with caution.

No proper investigation has been made of the efficiency of choosing to use a floating point precision (for all terms of the sum) based on the small size of the smallest y value.

No attempt has been made to translate into Lisp and compile the code to make timing trials for comparison purposes.

These (and other) refinements are left to the initiative of the hypothetical alert reader of limitless dedication (HAROLD).

## 9.3.4 The Gauss-Legendre Quadrature Method for $a \le x \le b$

Loosely quoting from David Bailey's slide presentations (see references at the end of the previous section)

The Gauss-Legendre quadrature method is an efficient method for continuous, well-behaved functions. In many cases, doubling the number of points at which the integrand is evaluated doubles the number of correct digits in the result. This method performs poorly for functions with algebraic and/or logarithmic end point singularities. The cost of computing the zeros of the Legendre polynomials and the corresponding "weights" increases as  $\mathbf{n}^2$  and thus becomes impractical for use beyond a few hundred digits.

Since one can always make a change of integration variable from the domain [a, b] to the integration domain [-1, 1], this method approximates an integral over [-1, 1] as the sum

$$\int_{-1}^{1} f(\mathbf{x}) \, d\mathbf{x} \approx \sum_{j=1}^{N} \mathbf{w_j} \, f(\mathbf{x_j}) \tag{9.19}$$

where the  $x_i$  are the roots of the N-th degree Legendre polynomial  $P_N(x)$  on [-1, 1], and the weights  $w_i$  are

$$w_{j} = \frac{-2}{(N+1) P'_{N}(x_{j}) P_{N+1}(x_{j})}$$
(9.20)

This method is implemented with our Ch.9 package file quad\_gs.mac, and Richard Fateman's lisp file:

```
http://www.cs.berkeley.edu/~fateman/generic/quad-maxima.lisp
```

which should be downloaded to use this package.

Except for the "driver" Maxima function quad\_gs (f,a,b,rp), all the Maxima functions in quad\_gs.mac are functions defined by Fateman in either the comment section of the above lisp file, or in the file http://www.cs.berkeley.edu/~fateman/papers/quadmax.mac.

An introduction to arbitrary precision code and some background to the problem of arbitrary precision quadrature has been provided by Richard Fateman in his draft paper **Numerical Quadrature in a Symbolic/Numerical Setting**, **quad.pdf** (see Sec. 9.2.6).

We will illustrate the available functions using the simple integral  $\int_{-1}^{1} e^{x} dx$ .

The package function **gaussunit**( $\mathbf{f}$ ,  $\mathbf{N}$ ) integrates the Maxima function  $\mathbf{f}$  over the domain [-1, 1] using  $\mathbf{N}$  point Gauss-Legendre quadrature.

```
(%i1) load("quad-maxima.lisp");
(%01)
                                quad-maxima.lisp
(%i2) fpprintprec:8$
(%i3) tval : bfloat(integrate(\exp(x), x, -1, 1)), fpprec:45;
                                    2.3504023b0
(%o3)
(%i4) load(quad_gs);
(%04)
                              c:/work3/quad_gs.mac
(%i5) arrays;
                                   [ab_and_wts]
(%05)
(%i6) arrayinfo(ab and wts);
                                    [hashed, 2]
(%06)
(%i7) gaussunit(exp,4);
                                   2.350402b0
(%07)
(%i8) abs(% - tval), fpprec:45;
                                  2.9513122b-7
(%08)
(%i9) fpprec;
                                        16
(%09)
(%i10) arrayinfo(ab_and_wts);
                              [hashed, 2, [4, 16]]
(%o10)
(%i11) first(ab_and_wts[4, 16]);
                          [8.6113631b-1, 3.3998104b-1]
(%o11)
(%i12) second( ab_and_wts[4, 16] );
(%o12)
                          [3.4785484b-1, 6.5214515b-1]
```

```
(%i13) lp4 : legenp(4,x);

4 2

35 x 15 x 3

(%o13) ----- + -

8 4 8

(%i14) float(solve(lp4));
(%o14) [x = -0.861136, x = 0.861136, x = -0.339981, x = 0.339981]
```

With the default value of **fpprec** = **16** and using only four integrand evaluation points, the error is about 2 parts in  $10^7$ . The first element of the two index hashed array **ab\_and\_wts[4,16]** is a list of the positive zeros of the fourth order Legendre polynomial  $P_4(x)$  (calculated with the arithmetic precision **fpprec** = **16**).

That fourth order Legendre polynomial  $P_4(x)$  can be displayed with this package using **legenp(4, x)**. Using **solve** we see that the roots for negative x are simply the positive roots with a minus sign, so the algorithm used makes use of this symmetry and keeps track of only the positive roots.

We can verify that the list of roots returned is correct to within the global floating point precision (we do this two different ways):

```
(%i15) lfp4(x) := legenp(4,x)$
(%i16) map('lfp4,%o11);
(%o16) [0.0b0, - 3.4694469b-18]
(%i17) map( lambda([z],legenp(4,z)),%o11 );
(%o17) [0.0b0, - 3.4694469b-18]
```

The second element of ab\_and\_wts[4,16] is a list of the weights which are associated with the positive roots (the negative roots have the same weights), with order corresponding to the order of the returned positive roots.

The package function <code>gaussunit\_e(f, N)</code> does the same job as <code>gaussunit(f, N)</code>, but returns a rough estimate of the amount contributed to the error by the floating point precision used (as the second element of a list:

```
(%i18) gaussunit_e(exp,4);
(%o18) [2.350402b0, 1.2761299b-17]
```

We see that the error attributable to the floating point precision used is insignificant compared to the error due to the low number of integrand evaluation points for this example.

An arbitrary finite integration interval is allowed with the functions gaussab(f, a, b, N) and gaussab(f, a, b, N) which use N point Gauss-Legendre quadrature over the interval [a, b], with the latter function being the analog of gaussunit\_e(f, N).

```
(%i19) gaussab(exp,-1,1,4);

(%o19) 2.350402b0

(%i20) abs(% - tval),fpprec:45;

(%o20) 2.9513122b-7

(%i21) gaussab_e(exp,-1,1,4);

(%o21) [2.350402b0, 1.2761299b-17]
```

The package function  $\mathbf{quad\_gs}$  (f, a, b, rp) integrates the Maxima function f over the finite interval [a,b], successively doubling the number of integrand evaluation points, stopping when the absolute value of the difference  $(I_n-I_{n/2})$  is less than  $10^{-\mathrm{rp}}$  (rp is the "requested precision" for the result), using the global setting of fpprec to use the corresponding precision arithmetic. We emphasize that Fateman's code uses a global setting of fpprec to achieve higher precision quadrature, rather that the method used in the previous two sections in which fpprec was set "locally" inside a block. This function returns the list

[ approx-value, number-function-evaluations, abs (vdiff) ], where the last element should be smaller than  $10^{-rp}$ .

Here we test this function for fpprec = 16, 30, and 40.

```
(%i22) quad_gs(exp,-1,1,10);
                                   fpprec = 16
(%o22)
                        [2.3504023b0, 20, 6.6613381b-16]
(%i23) abs(first(%) -tval),fpprec:45;
                                  6.2016267b-16
(%o23)
(%i24) fpprec:30$
(%i25) quad_gs(exp,-1,1,20);
                                   fpprec = 30
(%o25)
                        [2.3504023b0, 20, 1.2162089b-24]
(%i26) abs(first(%) -tval), fpprec:45;
                                  2.2001783b-30
(%o26)
(%i27) fpprec:40$
(%i28) quad_gs(exp,-1,1,30);
                                   fpprec = 40
                        [2.3504023b0, 40, 1.8367099b-40]
(%o28)
(%i29) abs(first(%) -tval), fpprec:45;
(%o29)
                                  2.7905177b-40
(%i30) gaussab_e(exp,-1,1,40);
                          [2.3504023b0, 1.8492214b-41]
(%o30)
```

We have checked the contribution to the error due to the forty digit arithmetic precision used, with N=40 point Gauss-Legendre quadrature (remember that N is the middle element of the list returned by

```
quad_gs (f, a, b, rp) and is also the last argument of the function gaussab_e(f, a, b, N).
```

We see that requesting **30** digit precision for the answer while using the global **fpprec** set to **40** results in an answer good to about **39** digits. Finally, let's check on what abscissae and weight arrays have been calculated so far:

```
(%i31) arrayinfo(ab_and_wts);
(%o31) [hashed, 2, [4, 16], [10, 16], [10, 30], [10, 40], [20, 16], [20, 30],
[20, 40], [40, 40]]
```

Using quad\_gs (f, a, b, rp) with fpprec = 16 led to the calculation of the abscissae and weight array for the index pairs [10,16] and [20,16] before the requested precision was achieved (the function always starts with N = 10 point quadrature and then successively doubles that number until success is achieved).

Using quad\_gs (f, a, b, rp) with fpprec = 30 led to the calculation of the abscissae and weight array for the index pairs [10, 30] and [20, 30] before the requested precision was achieved.

Using quad\_gs (f, a, b, rp) with fpprec = 40 led to the calculation of the abscissae and weight array for the index pairs [10, 40], [20, 40], and [40, 40] before the requested precision was achieved.

Finally, we have the function <code>quad\_gs\_table(f, a, b, rp)</code> which prints out a table showing the progression toward success:

(%i32) quad_gs_tak	ole(exp,-	l,1,30)\$	
		fpprec = 40	
new val	N	vdiff	
2.3504023b0	10		
2.3504023b0	20	1.2162183b-24	
2.3504023b0	40	1.8367099b-40	