GAIL—Guaranteed Automatic Integration Library in MATLAB: Documentation for Version 2.1*

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1 Introduction

Automatic and adaptive approximation, optimization, or integration of functions in a cone with guarantee of accuracy is a relatively new paradigm [7]. Our purpose is to create an open-source MATLAB package, Guaranteed Automatic Integration Library (GAIL) [5], following the philosophy of reproducible research championed by Claerbout [6] and Donoho [1], and sustainable practices of robust scientific software development [12]. For our conviction that true scholarship in computational sciences are characterized by reliable reproducibility [3, 4, 2], we employ the best practices in mathematical research and software engineering known to us and available in MATLAB.

The rest of this document describes the key features of functions in GAIL, which includes one-dimensional function approximation [7, 8] and minimization [14] using linear splines, one-dimensional numerical integration using trapezoidal rule [7], and last but not least, mean estimation and multidimensional integration by Monte Carlo methods [9, 11] or Quasi Monte Carlo methods [13, 10].

1.1 Downloads

GAIL can be downloaded from

http://code.google.com/p/gail/

Alternatively, you can get a local copy of the GAIL repository with this command:

git clone https://github.com/GailGithub/GAIL_Dev.git

1.2 Requirements

You will need to install MATLAB 7 or a later version.

1.3 Documentation

Detailed documentation is available at GAIL_Matlab/Documentation.

1.4 General Usage Notes

GAIL Version 2.1 [5] includes the following eight algorithms:

- 1. funappx_g [7, 8]: One-dimensional function approximation on bounded interval
- 2. funmin_g [14]: global minimum value of univariate function on a closed interval
- 3. integral_g [7]: One-dimensional integration on bounded interval
- 4. meanMC_{-g} [9]: Monte Carlo method for estimating mean of a random variable
- 5. meanMCBer_g [11]: Monte Carlo method to estimate the mean of a Bernoulli random variable
- 6. cubMC-g [9]: Monte Carlo method for numerical multiple integration
- 7. cubLattice_g [13]: Quasi-Monte Carlo method using rank-1 Lattices cubature for a d-dimensional integration
- 8. cubSobol_g [10]: Quasi-Monte Carlo method using Sobol' cubature for a d-dimensional integration

1.5 Installation Instruction

- 1. Unzip the contents of the zip file to a directory and maintain the existing directory and subdirectory structure. (Please note: If you install into the toolbox subdirectory of the MATLAB program hierarchy, you will need to click the button "Update toolbox path cache" from the File/Preferences... dialog in MATLAB.)
- 2. In MATLAB, add the GAIL directory to your path. This can be done by running GAIL_Install.m. Alternatively, this can be done by selecting "File/Set Path..." from the main or Command window menus, or with the command pathtool. We recommend that you select the "Save" button on this dialog so that GAIL is on the path automatically in future MATLAB sessions.
- 3. To check if you have installed GAIL successfully, type help funappx_g to see if its documentation shows up.

Alternatively, you could do this:

- 1. Download DownloadInstallGail_2_1.m and put it where you want GAIL to be installed.
- 2. Execute it in MATLAB.

To uninstall GAIL, execute GAIL_Uninstall.

To reinstall GAIL, execute GAIL_Install.

1.6 Tests

We provide quick doctests for each of the functions above. To run doctests in funappx_g, for example, issue the command doctest funappx_g.

We also provide unit tests for MATLAB version 8 or later. To run unit tests for funmin_g, for instance, execute run(ut_funmin_g).

1.7 Contact Information

Please send any queries, questions, or comments to

gail-users@googlegroups.com

1.8 Website

For more information about GAIL, visit GAIL Project website.

2 funappx_g

1-D guaranteed locally adaptive function approximation (or function recovery) on [a,b]

2.1 Syntax

```
fappx = funappx_g(f)

fappx = funappx_g(f,a,b,abstol)

fappx = funappx_g(f,'a',a,'b',b,'abstol',abstol)

fappx = funappx_g(f,in_param)

[fappx, out_param] = funappx_g(f,...)
```

2.2 Description

fappx = $funappx_g(f)$ approximates function f on the default interval [0,1] by an approximated function handle fappx within the guaranteed absolute error tolerance of 1e-6. When Matlab version is higher or equal to 8.3, fappx is an interpolant generated by griddedInterpolant. When Matlab version is lower than 8.3, fappx is a function handle generated by ppval and interp1. Input f is a function handle. The statement y = f(x) should accept a vector argument x and return a vector y of function values that is of the same size as x.

 $fappx = funappx_g(f,a,b,abstol)$ for a given function f and the ordered input parameters that define the finite interval [a,b], and a guaranteed absolute error tolerance abstol.

 $fappx = funappx_g(f, a, b, abstol, abstol)$ approximates function f on the finite interval [a,b], given a guaranteed absolute error tolerance abstol. All four field-value pairs are optional and can be supplied in different order.

fappx = **funappx**_**g**(f,in_param) approximates function f on the finite interval [in_param.a,in_param.b], given a guaranteed absolute error tolerance in_param.abstol. If a field is not specified, the default value is used.

 $[fappx, out_param] = funappx_g(f,...)$ returns an approximated function fappx and an output structure out_param.

Input Arguments

- f input function
- in_param.a left end point of interval, default value is 0
- in_param.b right end point of interval, default value is 1
- in_param.abstol guaranteed absolute error tolerance, default value is 1e-6

Optional Input Arguments

- in_param.nlo lower bound of initial number of points we used, default value is 10
- in_param.nhi upper bound of initial number of points we used, default value is 1000
- in_param.nmax when number of points hits the value, iteration will stop, default value is 1e7

• in_param.maxiter — max number of iterations, default value is 1000

Output Arguments

- fappx approximated function handle (Note: When Matlab version is higher or equal to 8.3, fappx is an interpolant generated by griddedInterpolant. When Matlab version is lower than 8.3, fappx is a function handle generated by ppval and interp1.)
- out_param.f input function
- out_param.a left end point of interval
- out_param.b right end point of interval
- $\bullet\,$ out_param.abstol guaranteed absolute error tolerance
- out_param.nlo a lower bound of initial number of points we use
- out_param.nhi an upper bound of initial number of points we use
- out_param.nmax when number of points hits the value, iteration will stop
- out_param.maxiter max number of iterations
- out_param.ninit initial number of points we use for each sub interval
- out_param.exit this is a number defining the conditions of success or failure satisfied when finishing the algorithm. The algorithm is considered successful (with out_param.exit == 0) if no other flags arise warning that the results are certainly not guaranteed. The initial value is 0 and the final value of this parameter is encoded as follows: 1 If reaching overbudget. It states whether the max budget is attained without reaching the guaranteed error tolerance.
 - 2 If reaching overiteration. It states whether the max iterations is attained without reaching the guaranteed error tolerance.
- out_param.iter number of iterations
- out_param.npoints number of points we need to reach the guaranteed absolute error tolerance
- out_param.errest an estimation of the absolute error for the approximation
- out_param.nstar final value of the parameter defining the cone of functions for which this algorithm is guaranteed for each subinterval; nstar = ninit-2 initially

2.3 Guarantee

For [a, b], there exists a partition

$$P = \{[t_0, t_1], [t_1, t_2], \dots, [t_{L-1}, t_L]\}, a = t_0 < t_1 < \dots < t_L = b.$$

If the function to be approximated, f satisfies the cone condition

$$||f''||_{\infty} \le \frac{2\text{nstar}}{t_l - t_{l-1}} \left| |f' - \frac{f(t_l) - f(t_{l-1})}{t_l - t_{l-1}} \right| |_{\infty}$$

for each sub interval $[t_{l-1}, t_l]$, where $1 \leq l \leq L$, then the fappx |output by this algorithm is guaranteed to satisfy

$$||f - fappx||_{\infty} \le abstol.$$

2.4 Examples

nmax: 10000000

Example 1

```
f = @(x) x.^2; [fappx, out_param] = funappx_g(f)
\% Approximate function x^2 with default input parameter to make the error
% less than 1e-6. For MATLAB version 8.3 onwards, we see:
fappx =
  griddedInterpolant with properties:
            GridVectors: {[1x3169 double]}
                 Values: [1x3169 double]
                 Method: 'linear'
    ExtrapolationMethod: 'linear'
out_param =
          f: @(x)x.^2
          a: 0
          b: 1
     abstol: 1.0000e-06
        nlo: 10
        nhi: 1000
       nmax: 10000000
    maxiter: 1000
      ninit: 100
       exit: [2x1 logical]
       iter: 6
    npoints: 3169
     errest: 2.7429e-07
      nstar: [1x32 double]
For earlier versions of MATLAB, we have:
fappx =
    @(x)ppval(pp,x)
out_param =
          f: @(x)x.^2
          a: 0
          b: 1
     abstol: 1.0000e-06
       nlo: 10
        nhi: 1000
```

maxiter: 1000 ninit: 100 exit: [2x1 logical] iter: 6 npoints: 3169 errest: 2.7429e-07 Example 2 [fappx, out_param] = $funappx_g(@(x) x.^2,0,100,1e-7,10,1000,1e8)$ % Approximate function x^2 on [0,100] with error tolerance 1e-7, cost % budget 10000000, lower bound of initial number of points 10 and upper % bound of initial number of points 100 fappx = griddedInterpolant with properties: GridVectors: {[1x977921 double]} Values: [1x977921 double] Method: 'linear' ExtrapolationMethod: 'linear' out_param = a: 0 abstol: 1.0000e-07 b: 100 $f: @(x)x.^2$ maxiter: 1000 nhi: 1000 nlo: 10 nmax: 100000000 ninit: 956 exit: [2x1 logical] iter: 11 npoints: 977921 errest: 3.7104e-08 nstar: [1x1024 double]

Example 3

```
clear in_param; in_param.a = -20; in_param.b = 20; in_param.nlo = 10;
in_param.nhi = 100; in_param.nmax = 1e8; in_param.abstol = 1e-7;
[fappx, out_param] = funappx_g(@(x) x.^2, in_param)
% Approximate function x^2 on [-20,20] with error tolerance 1e-7, cost
% budget 1000000, lower bound of initial number of points 10 and upper
\% bound of initial number of points 100
```

```
fappx =
  griddedInterpolant with properties:
            GridVectors: {[1x385025 double]}
                 Values: [1x385025 double]
                 Method: 'linear'
    ExtrapolationMethod: 'linear'
out_param =
          a: -20
     abstol: 1.0000e-07
          b: 20
          f: @(x)x.^2
    maxiter: 1000
       nhi: 100
        nlo: 10
       nmax: 100000000
     ninit: 95
       exit: [2x1 logical]
       iter: 13
    npoints: 385025
     errest: 2.6570e-08
      nstar: [1x4096 double]
Example 4
clear in_param; f = 0(x) x.^2;
[fappx, out_param] = funappx_g(f,'a',-10,'b',50,'nmax',1e6,'abstol',1e-7)
% Approximate function x^2 with error tolerance 1e-7, cost budget 1000000,
% lower bound of initial number of points 10 and upper
% bound of initial number of points 100
fappx =
  griddedInterpolant with properties:
            GridVectors: {[1x474625 double]}
                 Values: [1x474625 double]
                 Method: 'linear'
    ExtrapolationMethod: 'linear'
out_param =
          a: -10
     abstol: 1.0000e-07
          b: 50
          f: @(x)x.^2
    maxiter: 1000
```

nhi: 1000 nlo: 10 nmax: 1000000 ninit: 928

exit: [2x1 logical]

iter: 10
npoints: 474625
errest: 6.0849e-08
nstar: [1x512 double]

2.5 See Also

interp1, griddedInterpolant, integral_g, funmin_g, meanMC_g, cubMC_g

3 funmin_g

1-D guaranteed global minimum value on [a,b] and the subset containing optimal solutions

3.1 Syntax

```
fmin = funmin_g(f)
fmin = funmin_g(f,a,b,abstol,TolX)
fmin = funmin_g(f,'a',a,'b',b,'abstol',abstol,'TolX',TolX)
fmin = funmin_g(f,in_param)
[fmin, out_param] = funmin_g(f,...)
```

3.2 Description

fmin = $funmin_g(f)$ finds minimum value of function f on the default interval [0,1] within the guaranteed absolute error tolerance of 1e-6 and the X tolerance of 1e-3. Default initial number of points is 100 and default cost budget is 1e7. Input f is a function handle.

 $fmin = funmin_g(f,a,b,abstol,TolX)$ finds minimum value of function f with ordered input parameters that define the finite interval [a,b], a guaranteed absolute error tolerance abstol and a guaranteed X tolerance TolX.

 $fmin = funmin_g(f, a, b, a)$ by by a guaranteed $fmin = funmin_g(f, a, b)$, abstol, abstol, $fmin = funmin_g(f, a, b)$, with a guaranteed absolute error tolerance abstol and a guaranteed fmin = function f to the interval $fmin = funmin_g(f, a, b)$, with a guaranteed absolute error tolerance abstol and a guaranteed $fmin = funmin_g(f, a, a, b, b)$, abstol, $fmin = funmin_g(f, a, a, b)$, and $fmin = funmin_g(f, a, a,$

 $fmin = funmin_g(f,in_param)$ finds minimum value of function f on the interval [in_param.a,in_param.b] with a guaranteed absolute error tolerance in_param.abstol and a guaranteed X tolerance in_param.TolX. If a field is not specified, the default value is used.

 $[fmin, out_param] = funmin_g(f,...)$ returns minimum value fmin of function f and an output structure out_param.

Input Arguments

- f input function
- in_param.a left end point of interval, default value is 0
- in_param.b right end point of interval, default value is 1
- in_param.abstol guaranteed absolute error tolerance, default value is 1e-6.
- in_param.TolX guaranteed X tolerance, default value is 1e-3.

Optional Input Arguments

- in_param.nlo lower bound of initial number of points we used, default value is 10
- in_param.nhi upper bound of initial number of points we used, default value is 1000

• in_param.nmax — cost budget, default value is 1e7.

Output Arguments

- out_param.f input function
- out_param.a left end point of interval
- out_param.b right end point of interval
- out_param.abstol guaranteed absolute error tolerance
- out_param.TolX guaranteed X tolerance
- out_param.nlo a lower bound of initial number of points we use
- out_param.nhi an upper bound of initial number of points we use
- out_param.nmax cost budget
- out_param.ninit initial number of points we use
- out_param.tau latest value of tau
- out_param.npoints number of points needed to reach the guaranteed absolute error tolerance or the guaranteed X tolerance
- out_param.exitflag the state of program when exiting
 - 0 Success
 - 1 Number of points used is greater than out_param.nmax
- out_param.errest estimation of the absolute error bound
- out_param.volumeX the volume of intervals containing the point(s) where the minimum occurs
- out_param.tauchange it is 1 if out_param.tau changes, otherwise it is 0
- out_param.intervals the intervals containing point(s) where the minimum occurs. Each column indicates one interval where the first row is the left point and the second row is the right point.

3.3 Guarantee

If the function to be minimized, f satisfies the cone condition

$$||f''||_{\infty} \le \frac{\tau}{b-a} \left| |f' - \frac{f(b) - f(a)}{b-a} \right||_{\infty},$$

then the fmin output by this algorithm is guaranteed to satisfy

$$|\min f - \min| \le \text{abstol},$$

or

$$volumeX < TolX$$
,

provided the flag exitflag = 0.

3.4 Examples

Example 1

```
f=0(x) (x-0.3).^2+1; [fmin,out_param] = funmin_g(f)
\% Minimize function (x-0.3)^2+1 with default input parameter.
fmin =
    1.0000
out_param =
            f: @(x)(x-0.3).^2+1
            a: 0
            b: 1
       abstol: 1.0000e-06
         TolX: 1.0000e-03
         nlo: 10
         nhi: 1000
         nmax: 10000000
        ninit: 100
          tau: 197
     exitflag: 0
      npoints: 6337
       errest: 6.1554e-07
      volumeX: 0.0015
    tauchange: 0
    intervals: [2x1 double]
Example 2
f=0(x) (x-0.3).^2+1;
[fmin,out\_param] = funmin\_g(f,-2,2,1e-7,1e-4,10,10,1000000)
\% Minimize function (x-0.3)^2+1 on [-2,2] with error tolerance 1e-4, X
\% tolerance 1e-2, cost budget 1000000, lower bound of initial number of
% points 10 and upper bound of initial number of points 10
fmin =
    1.0000
out_param =
            a: -2
       abstol: 1.0000e-07
            b: 2
            f: @(x)(x-0.3).^2+1
```

```
nhi: 10
         nlo: 10
        nmax: 1000000
        TolX: 1.0000e-04
       ninit: 10
          tau: 17
     exitflag: 0
     npoints: 18433
      errest: 9.5464e-08
     volumeX: 5.4175e-04
   tauchange: 0
    intervals: [2x1 double]
Example 3
clear in_param; in_param.a = -13; in_param.b = 8;
in_param.abstol = 1e-7; in_param.TolX = 1e-4;
in_param.nlo = 10; in_param.nhi = 100;
in_param.nmax = 10^6;
[fmin,out_param] = funmin_g(f,in_param)
\% Minimize function (x-0.3)^2+1 on [-13,8] with error tolerance 1e-7, X
\% tolerance 1e-4, cost budget 1000000, lower bound of initial number of
% points 10 and upper bound of initial number of points 100
fmin =
     1
out_param =
           a: -13
      abstol: 1.0000e-07
           b: 8
           f: @(x)(x-0.3).^2+1
         nhi: 100
         nlo: 10
         nmax: 1000000
        TolX: 1.0000e-04
       ninit: 91
          tau: 179
     exitflag: 0
     npoints: 368641
      errest: 7.1014e-08
      volumeX: 5.2445e-04
   tauchange: 0
    intervals: [2x1 double]
```

Example 4

```
f=0(x) (x-0.3).^2+1;
[fmin,out_param] = funmin_g(f,'a',-2,'b',2,'nhi',100,'nlo',10,...
    'nmax',1e6,'abstol',1e-4,'TolX',1e-2)
\% Minimize function (x-0.3)^2+1 on [-2,2] with error tolerance 1e-4, X
% tolerance 1e-2, cost budget 1000000, lower bound of initial number of
\% points 10 and upper bound of initial number of points 100
fmin =
    1.0000
out_param =
           a: -2
       abstol: 1.0000e-04
           b: 2
           f: @(x)(x-0.3).^2+1
         nhi: 100
         nlo: 10
         nmax: 1000000
        TolX: 0.0100
        ninit: 64
          tau: 125
     exitflag: 0
     npoints: 2017
       errest: 6.2273e-05
      volumeX: 0.0146
    tauchange: 0
    intervals: [2x1 double]
```

3.5 See Also

fminbnd, funappx_g, integral_g

4 integral_g

1-D guaranteed function integration using trapezoidal rule

4.1 Syntax

```
q = integral\_g(f)
q = integral\_g(f,a,b,abstol)
q = integral\_g(f,'a',a,'b',b,'abstol',abstol)
q = integral\_g(f,in\_param)
[q, out\_param] = integral\_g(f,...)
```

4.2 Description

 $q = integral_g(f)$ computes q, the definite integral of function f on the interval [a,b] by trapezoidal rule with in a guaranteed absolute error of 1e-6. Default starting number of sample points taken is 100 and default cost budget is 1e7. Input f is a function handle. The function y = f(x) should accept a vector argument x and return a vector result y, the integrand evaluated at each element of x.

 $q = integral_g(f,a,b,abstol)$ computes q, the definite integral of function f on the finite interval [a,b] by trapezoidal rule with the ordered input parameters, and guaranteed absolute error tolerance abstol.

 $q = integral_g(f, a', a, b', b, abstol', abstol')$ computes q, the definite integral of function f on the finite interval [a,b] by trapezoidal rule within a guaranteed absolute error tolerance abstol. All four field-value pairs are optional and can be supplied.

 $q = integral_g(f,in_param)$ computes q, the definite integral of function f by trapezoidal rule within a guaranteed absolute error in_param.abstol. If a field is not specified, the default value is used.

[q, out_param] = integral_g(f,...) returns the approximated integration q and output structure out_param.

Input Arguments

- f input function
- in_param.a left end of the integral, default value is 0
- in_param.b right end of the integral, default value is 1
- in_param.abstol guaranteed absolute error tolerance, default value is 1e-6

Optional Input Arguments

- in_param.nlo lowest initial number of function values used, default value is 10
- in-param.nhi highest initial number of function values used, default value is 1000
- in_param.nmax cost budget (maximum number of function values), default value is 1e7
- in_param.maxiter max number of iterations, default value is 1000

Output Arguments

- q approximated integral
- out_param.f input function
- out_param.a low end of the integral
- out_param.b high end of the integral
- out_param.abstol guaranteed absolute error tolerance
- out_param.nlo lowest initial number of function values
- $\bullet\,$ out_param.nhi highest initial number of function values
- out_param.nmax cost budget (maximum number of function values)
- out_param.maxiter max number of iterations
- out_param.ninit initial number of points we use, computed by nlo and nhi
- out_param.tauchange it is true if the cone constant has been changed, false otherwise. See [1] for details. If true, you may wish to change the input in_param.ninit to a larger number.
- out_param.tauchange it is true if the cone constant has been changed, false otherwise. See [1] for details. If true, you may wish to change the input in_param.ninit to a larger number.
- out_param.iter number of iterations
- out_param.npoints number of points we need to reach the guaranteed absolute error tolerance abstol.
- out_param.errest approximation error defined as the differences between the true value and the approximated value of the integral.
- out_param.nstar final value of the parameter defining the cone of functions for which this algorithm is guaranteed; nstar = ninit-2 initially and is increased as necessary
- out_param.exit the state of program when exiting
 - 0 Success
 - 1 Number of points used is greater than out_param.nmax
 - 2 Number of iterations is greater than out_param.maxiter

4.3 Guarantee

If the function to be integrated, f satisfies the cone condition

$$||f''||_1 \le \frac{\text{nstar}}{2(b-a)} ||f' - \frac{f(b) - f(a)}{b-a}||_1$$

then the q output by this algorithm is guaranteed to satisfy

$$\left\| \int_{a}^{b} f(x)dx - q \right\|_{1} \le \text{abstol},$$

provided the flag exceedbudget = 0. And the upper bound of the cost is

$$\sqrt{\frac{\operatorname{nstar}*(b-a)^2\operatorname{Var}(f')}{2\times\operatorname{abstol}}} + 2\times\operatorname{nstar} + 4.$$

4.4 Examples

Example 1

```
f = @(x) x.^2; [q, out\_param] = integral_g(f)
% than 1e-7.
q =
   0.3333
out_param =
             f: @(x)x.^2
             a: 0
             b: 1
         abstol: 1.0000e-06
           nlo: 10
           nhi: 1000
          nmax: 10000000
        maxiter: 1000
          ninit: 100
           tau: 197
   exceedbudget: 0
      tauchange: 0
           iter: 2
             q: 0.3333
        npoints: 3565
         errest: 9.9688e-07
Example 2
[q, out_param] = integral_g(@(x) \exp(-x.^2), 'a',1,'b',2,...
   'nlo',100,'nhi',10000,'abstol',1e-5,'nmax',1e7)
% Integrate function x^2 with starting number of points 52, cost budget
\% 10000000 and error tolerance 1e-8
q =
   0.1353
out_param =
             a: 1
         abstol: 1.0000e-05
             b: 2
             f: @(x) exp(-x.^2)
        maxiter: 1000
```

nhi: 10000 nlo: 100 nmax: 10000000 ninit: 1000

tau: 1997 exceedbudget: 0

tauchange: 0
 iter: 2

q: 0.1353 npoints: 2998

errest: 7.3718e-06

4.5 See Also

integral, quad, funappx_g, meanMC_g, cubMC_g, funmin_g

5 meanMC₋g

Monte Carlo method to estimate the mean of a random variable

5.1 Syntax

```
\begin{split} &tmu = \mathbf{meanMC\_g}(Yrand) \\ &tmu = \mathbf{meanMC\_g}(Yrand,abstol,reltol,alpha) \\ &tmu = \mathbf{meanMC\_g}(Yrand,'abstol',abstol,'reltol',reltol,'alpha',alpha) \\ &[tmu, out\_param] = \mathbf{meanMC\_g}(Yrand,in\_param) \end{split}
```

5.2 Description

 $tmu = meanMC_g(Yrand)$ estimates the mean, mu, of a random variable Y to within a specified generalized error tolerance, tolfun:=max(abstol,reltol*| mu |), i.e., | mu - tmu | <= tolfun with probability at least 1-alpha, where abstol is the absolute error tolerance, and reltol is the relative error tolerance. Usually the reltol determines the accuracy of the estimation, however, if the | mu | is rather small, the abstol determines the accuracy of the estimation. The default values are abstol=1e-2, reltol=1e-1, and alpha=1%. Input Yrand is a function handle that accepts a positive integer input n and returns an n x 1 vector of IID instances of the random variable Y.

tmu = meanMC_g(Yrand,abstol,reltol,alpha) estimates the mean of a random variable Y to within a specified generalized error tolerance tolfun with guaranteed confidence level 1-alpha using all ordered parsing inputs abstol, reltol, alpha.

 $tmu = meanMC_g(Yrand, 'abstol', abstol', 'reltol', 'reltol', 'alpha', alpha')$ estimates the mean of a random variable Y to within a specified generalized error tolerance tolfun with guaranteed confidence level 1-alpha. All the field-value pairs are optional and can be supplied in different order, if a field is not supplied, the default value is used.

 $[tmu, out_param] = meanMC_g(Yrand,in_param)$ estimates the mean of a random variable Y to within a specified generalized error tolerance tolfun with the given parameters in_param and produce the estimated mean tmu and output parameters out_param. If a field is not specified, the default value is used.

Input Arguments

- Yrand the function for generating n IID instances of a random variable Y whose mean we want to estimate. Y is often defined as a function of some random variable X with a simple distribution. The input of Yrand should be the number of random variables n, the output of Yrand should be n function values. For example, if $Y = X.^2$ where X is a standard uniform random variable, then one may define Yrand = @(n) rand(n,1).^2.
- in_param.abstol the absolute error tolerance, which should be positive, default value is 1e-2.
- in_param.reltol the relative error tolerance, which should be between 0 and 1, default value is 1e-1.
- in_param.alpha the uncertainty, which should be a small positive percentage. default value is 1%.

Optional Input Arguments

• in_param.fudge — standard deviation inflation factor, which should be larger than 1, default value is 1.2.

- in_param.nSig initial sample size for estimating the sample variance, which should be a moderate large integer at least 30, the default value is 1e4.
- in_param.n1 initial sample size for estimating the sample mean, which should be a moderate large positive integer at least 30, the default value is 1e4.
- in_param.tbudget the time budget in seconds to do the two-stage estimation, which should be positive, the default value is 100 seconds.
- in_param.nbudget the sample budget to do the two-stage estimation, which should be a large positive integer, the default value is 1e9.

Output Arguments

- tmu the estimated mean of Y.
- out_param.tau the iteration step.
- out_param.n the sample size used in each iteration.
- out_param.nremain the remaining sample budget to estimate mu. It was calculated by the sample left and time left.
- out_param.ntot total sample used.
- out_param.hmu estimated mean in each iteration.
- out_param.tol the reliable upper bound on error for each iteration.
- out_param.var the sample variance.
- out_param.exit the state of program when exiting.
 - 0 Success
 - 1 Not enough samples to estimate the mean
- out_param.kurtmax the upper bound on modified kurtosis.
- out_param.time the time elapsed in seconds.
- out_param.flag parameter checking status
 - 1 checked by meanMC_g

5.3 Guarantee

This algorithm attempts to calculate the mean, mu, of a random variable to a prescribed error tolerance, tolfun:= $\max(\text{abstol,reltol*}|\text{ mu }|)$, with guaranteed confidence level 1-alpha. If the algorithm terminated without showing any warning messages and provide an answer tmu, then the follow inequality would be satisfied: $\Pr(|\text{ mu - tmu }| <= \text{tolfun}) >= 1$ -alpha The cost of the algorithm, N₋tot, is also bounded above

by N_{up} , which is defined in terms of abstol, reltol, nSig, n1, fudge, kurtmax, beta. And the following inequality holds: $Pr(N_{tot} \le N_{up}) >= 1$ -beta Please refer to our paper for detailed arguments and proofs.

5.4 Examples

Example 1

```
% Calculate the mean of x^2 when x is uniformly distributed in
\% [O 1], with the absolute error tolerance = 1e-3 and uncertainty 5\%.
  in_param.reltol=0; in_param.abstol = 1e-3;in_param.reltol = 0;
  in_param.alpha = 0.05; Yrand=0(n) rand(n,1).^2;
  tmu = meanMC_g(Yrand,in_param)
tmu =
    0.3331
Example 2
% Calculate the mean of exp(x) when x is uniformly distributed in
\% [O 1], with the absolute error tolerance 1e-3.
  tmu = meanMC_g(@(n)exp(rand(n,1)), 1e-3,0)
tmu =
    1.7185
Example 3
% Calculate the mean of cos(x) when x is uniformly distributed in
\% [0 1], with the relative error tolerance 1e-2 and uncertainty 0.05.
  tmu = meanMC_g(@(n)cos(rand(n,1)), 'reltol', 1e-2, 'abstol', 0, ...
      'alpha',0.05)
tmu =
    0.8415
```

5.5 See Also

funappx_g, integral_g, cubMC_g, meanMCBer_g, cubSobol_g, cubLattice_g

6 meanMCBer_g

Monte Carlo method to estimate the mean of a Bernoulli random variable to within a specified absolute error tolerance with guaranteed confidence level 1-alpha.

6.1 Syntax

```
pHat = meanMCBer_g(Yrand)

pHat = meanMCBer_g(Yrand,abstol,alpha,nmax)

pHat = meanMCBer_g(Yrand,'abstol',abstol,'alpha',alpha,'nmax',nmax)

[pHat, out_param] = meanMCBer_g(Yrand,in_param)
```

6.2 Description

pHat = meanMCBer_g(Yrand) estimates the mean of a Bernoulli random variable Y to within a specified absolute error tolerance with guaranteed confidence level 99%. Input Yrand is a function handle that accepts a positive integer input n and returns a n x 1 vector of IID instances of the Bernoulli random variable Y.

pHat = meanMCBer_g(Yrand,abstol,alpha,nmax) estimates the mean of a Bernoulli random variable Y to within a specified absolute error tolerance with guaranteed confidence level 1-alpha using all ordered parsing inputs abstol, alpha and nmax.

pHat = meanMCBer_g(Yrand,'abstol',abstol,'alpha',alpha,'nmax',nmax) estimates the mean of a Bernoulli random variable Y to within a specified absolute error tolerance with guaranteed confidence level 1-alpha. All the field-value pairs are optional and can be supplied in different order.

[pHat, out_param] = meanMCBer_g(Yrand,in_param) estimates the mean of a Bernoulli random variable Y to within a specified absolute error tolerance with the given parameters in_param and produce the estimated mean pHat and output parameters out_param.

Input Arguments

- Yrand the function for generating IID instances of a Bernoulli random variable Y whose mean we want to estimate.
- pHat the estimated mean of Y.
- in_param.abstol the absolute error tolerance, the default value is 1e-2.
- in_param.alpha the uncertainty, the default value is 1%.
- in_param.nmax the sample budget, the default value is 1e9.

Output Arguments

- out_param.n the total sample used.
- out_param.time the time elapsed in seconds.
- out_param.exit the state of program when exiting.
 - 0 Success
 - 1 Not enough samples to estimate p with guarantee

6.3 Guarantee

If the sample size is calculated according Hoeffding's inequality, which equals to $\operatorname{ceil}(\log(2/\operatorname{out_param.alpha})/(2*\operatorname{out_param.abstol}^2))$, then the following inequality must be satisfied: $\Pr(\mid p - pHat \mid <= abstol) >= 1-alpha$. Here p is the true mean of Yrand, and pHat is the output of

MEANMCBER_G. Also, the cost is deterministic.

6.4 Examples

Example 1

```
% Calculate the mean of a Bernoulli random variable with true p=1/90,
% absolute error tolerance 1e-3 and uncertainty 0.01.
    in_param.abstol=1e-3; in_param.alpha = 0.01; in_param.nmax = 1e9;
    p=1/9; Yrand=@(n) rand(n,1)<p;</pre>
    pHat = meanMCBer_g(Yrand,in_param)
pHat =
    0.1113
Example 2
% Using the same function as example 1, with the absolute error tolerance
% 1e-4.
    pHat = meanMCBer_g(Yrand, 1e-4)
pHat =
    0.1111
Example 3
% Using the same function as example 1, with the absolute error tolerance
\% 1e-2 and uncertainty 0.05.
    pHat = meanMCBer_g(Yrand, 'abstol', 1e-2, 'alpha', 0.05)
pHat =
    0.1118
```

6.5 See Also

funappx_g, integral_g, cubMC_g, meanMC_g, cubLattice_g, cubSobol_g

7 cubMC_g

Monte Carlo method to evaluate a multidimensional integral

7.1 Syntax

```
[Q,out\_param] = \mathbf{cubMC\_g}(f,hyperbox)
Q = \mathbf{cubMC\_g}(f,hyperbox,measure,abstol,reltol,alpha)
Q = \mathbf{cubMC\_g}(f,hyperbox,'measure',measure,'abstol',abstol,'reltol',reltol,'alpha',alpha)
[Q out\_param] = \mathbf{cubMC\_g}(f,hyperbox,in\_param)
```

7.2 Description

[Q,out_param] = $\operatorname{cubMC_g}(f, \operatorname{hyperbox})$ estimates the integral of f over hyperbox to within a specified generalized error tolerance, tolfun = $\max(\operatorname{abstol}, \operatorname{reltol}^* | I |)$, i.e., $| I - Q | <= \operatorname{tolfun}$ with probability at least 1-alpha, where abstol is the absolute error tolerance, and reltol is the relative error tolerance. Usually the reltol determines the accuracy of the estimation, however, if the | I | is rather small, the abstol determines the accuracy of the estimation. The default values are abstol=1e-2, reltol=1e-1, and alpha=1%. Input f is a function handle that accepts an n x d matrix input, where d is the dimension of the hyperbox, and n is the number of points being evaluated simultaneously. The input hyperbox is a 2 x d matrix, where the first row corresponds to the lower limits and the second row corresponds to the upper limits.

 $Q = \text{cubMC_g}(f, \text{hyperbox}, \text{measure}, \text{abstol}, \text{reltol}, \text{alpha})$ estimates the integral of function f over hyperbox to within a specified generalized error tolerance tolfun with guaranteed confidence level 1-alpha using all ordered parsing inputs f, hyperbox, measure, abstol, reltol, alpha, fudge, nSig, n1, tbudget, nbudget, flag. The input f and hyperbox are required and others are optional.

 $Q = \mathbf{cubMC_g}(f, hyperbox, 'measure', measure', abstol', abstol', reltol', reltol', reltol', alpha', alpha) estimates the integral of f over hyperbox to within a specified generalized error tolerance tolfun with guaranteed confidence level 1-alpha. All the field-value pairs are optional and can be supplied in different order. If an input is not specified, the default value is used.$

[Q out_param] = **cubMC**_g(f,hyperbox,in_param) estimates the integral of f over hyperbox to within a specified generalized error tolerance tolfun with the given parameters in_param and produce output parameters out_param and the integral Q.

Input Arguments

- f the integrand.
- hyperbox the integration hyperbox. The default value is [zeros(1,d); ones(1,d)], the default d is 1.
- in_param.measure the measure for generating the random variable, the default is 'uniform'. The other measure could be handled is 'normal'/'Gaussian'. The input should be a string type, hence with quotes.
- in_param.abstol the absolute error tolerance, the default value is 1e-2.
- in_param.reltol the relative error tolerance, the default value is 1e-1.
- in_param.alpha the uncertainty, the default value is 1%.

Optional Input Arguments

- in_param.fudge the standard deviation inflation factor, the default value is 1.2.
- in_param.nSig initial sample size for estimating the sample variance, which should be a moderate large integer at least 30, the default value is 1e4.
- in_param.n1 initial sample size for estimating the sample mean, which should be a moderate large positive integer at least 30, the default value is 1e4.
- in_param.tbudget the time budget to do the estimation, the default value is 100 seconds.
- in_param.nbudget the sample budget to do the estimation, the default value is 1e9.
- in_param.flag the value corresponds to parameter checking status.
 - 0 not checked
 - 1 checked by meanMC_g
 - 2 checked by cubMC_g

Output Arguments

- Q the estimated value of the integral.
- out_param.n the sample size used in each iteration.
- out_param.ntot total sample used.
- out_param.nremain the remaining sample budget to estimate I. It was calculated by the sample left and time left.
- $\bullet\,$ out_param.tau the iteration step.
- out_param.hmu estimated integral in each iteration.
- out_param.tol the reliable upper bound on error for each iteration.
- out_param.kurtmax the upper bound on modified kurtosis.
- out_param.time the time elapsed in seconds.
- out_param.var the sample variance.
- out_param.exit the state of program when exiting.
 - 0 success
 - 1 Not enough samples to estimate the mean
 - 10 hyperbox does not contain numbers
 - 11 hyperbox is not 2 x d
 - 12 hyperbox is only a point in one direction
 - 13 hyperbox is infinite when measure is 'uniform'
 - 14 hyperbox is not doubly infinite when measure is 'normal'

7.3 Guarantee

This algorithm attempts to calculate the integral of function f over a hyperbox to a prescribed error tolerance tolfun:= $\max(abstol, reltol^*|I|)$ with guaranteed confidence level 1-alpha. If the algorithm terminated without showing any warning messages and provide an answer Q, then the follow inequality would be satisfied:

```
Pr(|Q - I| \le tolfun) >= 1-alpha
```

The cost of the algorithm, N_{tot}, is also bounded above by N_{up}, which is a function in terms of abstol, reltol, nSig, n1, fudge, kurtmax, beta. And the following inequality holds:

```
Pr (N_{tot} \le N_{up}) >= 1-beta
```

Please refer to our paper for detailed arguments and proofs.

in_param.abstol = 1e-3; in_param.reltol=1e-3;

Q = cubMC_g(f,hyperbox,in_param)

7.4 Examples

Example 1

```
% Estimate the integral with integrand f(x) = \sin(x) over the interval
% [1;2]
f = O(x) \sin(x); interval = [1;2];
Q = cubMC_g(f,interval,'uniform',1e-3,1e-2)
0 =
    0.9564
Example 2
% Estimate the integral with integrand f(x) = \exp(-x1^2-x2^2) over the
% hyperbox [0\ 0;1\ 1], where x is a vector x = [x1\ x2].
f = 0(x) \exp(-x(:,1).^2-x(:,2).^2); \text{ hyperbox} = [0 0;1 1];
Q = cubMC_g(f,hyperbox,'measure','uniform','abstol',1e-3,...
     'reltol',1e-13)
Q =
    0.5574
Example 3
% Estimate the integral with integrand f(x) = 2^d*prod(x1*x2*...*xd) +
\% 0.555 over the hyperbox [zeros(1,d);ones(1,d)], where x is a vector x =
% [x1 x2... xd].
  d = 3; f = Q(x) 2^d*prod(x,2)+0.555; hyperbox = [zeros(1,d); ones(1,d)];
```

```
Q =
    1.5549

Example 4

% Estimate the integral with integrand f(x) = exp(-x1^2-x2^2) in the % hyperbox [-inf -inf;inf inf], where x is a vector x = [x1 x2].

f = @(x) exp(-x(:,1).^2-x(:,2).^2); hyperbox = [-inf -inf;inf inf];
Q = cubMC_g(f,hyperbox,'normal',0,1e-2)

ans =
    1

Q =
```

7.5 See Also

0.3330

funappx_g, integral_g, meanMC_g, meanMCBer_g, cubLattice_g, cubSobol_g

8 cubLattice_g

Quasi-Monte Carlo method using rank-1 Lattices cubature over a d-dimensional region to integrate within a specified generalized error tolerance with guarantees under Fourier coefficients cone decay assumptions.

8.1 Syntax

```
[q,out_param] = cubLattice_g(f,hyperbox)

q = cubLattice_g(f,hyperbox,measure,abstol,reltol)

q = cubLattice_g(f,hyperbox,'measure',measure,'abstol',abstol,'reltol',reltol)

q = cubLattice_g(f,hyperbox,in_param)
```

8.2 Description

[q,out_param] = $\operatorname{cubLattice_g}(f, \operatorname{hyperbox})$ estimates the integral of f over the d-dimensional region described by hyperbox, and with an error guaranteed not to be greater than a specific generalized error tolerance, tolfun:=max(abstol,reltol*| integral(f) |). Input f is a function handle. f should accept an n x d matrix input, where d is the dimension and n is the number of points being evaluated simultaneously. The input hyperbox is a 2 x d matrix, where the first row corresponds to the lower limits and the second row corresponds to the upper limits of the integral. Given the construction of our Lattices, d must be a positive integer with 1 < = d < = 250.

q = cubLattice_g(f,hyperbox,measure,abstol,reltol) estimates the integral of f over the hyperbox. The answer is given within the generalized error tolerance tolfun. All parameters should be input in the order specified above. If an input is not specified, the default value is used. Note that if an input is not specified, the remaining tail cannot be specified either. Inputs f and hyperbox are required. The other optional inputs are in the correct order: measure,abstol,reltol,shift,mmin,mmax,fudge,transform,toltype and theta.

 $q = cubLattice_g(f,hyperbox,'measure',measure',abstol',abstol,'reltol',reltol')$ estimates the integral of f over the hyperbox. The answer is given within the generalized error tolerance tolfun. All the field-value pairs are optional and can be supplied in any order. If an input is not specified, the default value is used.

 $q = \mathbf{cubLattice}_{-\mathbf{g}}(f, hyperbox, in_param)$ estimates the integral of f over the hyperbox. The answer is given within the generalized error tolerance tolfun.

Input Arguments

- f the integrand whose input should be a matrix n x d where n is the number of data points and d the dimension, which cannot be greater than 250. By default f is f=@ x.^2.
- hyperbox the integration region defined by its bounds. It must be a 2 x d matrix, where the first row corresponds to the lower limits and the second row corresponds to the upper limits of the integral. The default value is [0;1].
- in_param.measure for f(x)*mu(dx), we can define mu(dx) to be the measure of a uniformly distributed random variable in they hyperbox or normally distributed with covariance matrix I_d. The only possible values are 'uniform' or 'normal'. For 'uniform', the hyperbox must be a finite volume while for 'normal', the hyperbox can only be defined as (-Inf,Inf)^d. By default it is 'uniform'.
- in_param.abstol the absolute error tolerance, abstol>=0. By default it is 1e-4.
- in_param.reltol the relative error tolerance, which should be in [0,1]. Default value is 1e-2.

Optional Input Arguments

- in_param.shift the Rank-1 lattices can be shifted to avoid the origin or other particular points. By default we consider a uniformly [0,1) random shift.
- in_param.mmin the minimum number of points to start is 2^mmin. The cone condition on the Fourier coefficients decay requires a minimum number of points to start. The advice is to consider at least mmin=10. mmin needs to be a positive integer with mmin<=mmax. By default it is 10.
- in_param.mmax the maximum budget is 2^mmax. By construction of our Lattices generator, mmax is a positive integer such that mmin<=mmax<=26. The default value is 24.
- in_param.fudge the positive function multiplying the finite sum of Fast Fourier coefficients specified in the cone of functions. This input is a function handle. The fudge should accept an array of nonnegative integers being evaluated simultaneously. For more technical information about this parameter, refer to the references. By default it is @(m) 5*2.^-m.
- in_param.transform the algorithm is defined for continuous periodic functions. If the input function f is not, there are 5 types of transform to periodize it without modifying the result. By default it is the Baker's transform. The options are:

'id': no transformation.

'Baker': Baker's transform or tent map in each coordinate. Preserving only continuity but simple to compute. Chosen by default.

'C0': polynomial transformation only preserving continuity.

'C1': polynomial transformation preserving the first derivative.

'C1sin': Sidi's transform with sine, preserving the first derivative. This is in general a better option than 'C1'.

- in_param.toltype this is the generalized tolerance function. There are two choices, 'max' which takes max(abstol,reltol*| integral(f) |) and 'comb' which is the linear combination theta*abstol+(1-theta)*reltol*| integral(f) | . Theta is another parameter to be specified with 'comb'(see below). For pure absolute error, either choose 'max' and set reltol = 0 or choose 'comb' and set theta = 1. For pure relative error, either choose 'max' and set abstol = 0 or choose 'comb' and set theta = 0. Note that with 'max', the user can not input abstol = reltol = 0 and with 'comb', if theta = 1 abstol con not be 0 while if theta = 0, reltol can not be 0. By default toltype is 'max'.
- in_param.theta this input is parametrizing the toltype 'comb'. Thus, it is only active when the toltype chosen is 'comb'. It establishes the linear combination weight between the absolute and relative tolerances theta*abstol+(1-theta)*reltol*| integral(f) |. Note that for theta = 1, we have pure absolute tolerance while for theta = 0, we have pure relative tolerance. By default, theta=1.

Output Arguments

- q the estimated value of the integral.
- out_param.d dimension over which the algorithm integrated.
- out_param.n number of Rank-1 lattice points used for computing the integral of f.
- out_param.bound_err predicted bound on the error based on the cone condition. If the function lies in the cone, the real error will be smaller than generalized tolerance.
- out_param.time time elapsed in seconds when calling cubLattice_g.

- out_param.exitflag this is a binary vector stating whether warning flags arise. These flags tell about which conditions make the final result certainly not guaranteed. One flag is considered arisen when its value is 1. The following list explains the flags in the respective vector order:
 - 1 If reaching overbudget. It states whether the max budget is attained without reaching the guaranteed error tolerance.
 - 2 If the function lies outside the cone. In this case, results are not guaranteed. Note that this parameter is computed on the transformed function, not the input function. For more information on the transforms, check the input parameter in_param.transform; for information about the cone definition, check the article mentioned below.

8.3 Guarantee

This algorithm computes the integral of real valued functions in dimension d with a prescribed generalized error tolerance. The Fourier coefficients of the integrand are assumed to be absolutely convergent. If the algorithm terminates without warning messages, the output is given with guarantees under the assumption that the integrand lies inside a cone of functions. The guarantee is based on the decay rate of the Fourier coefficients. For more details on how the cone is defined, please refer to the references below.

8.4 Examples

Example 1

```
% Estimate the integral with integrand f(x) = x1.*x2 in the interval
% [0,1)^2:
 f = Q(x) \operatorname{prod}(x,2); hyperbox = [zeros(1,2); ones(1,2)];
  q = cubLattice_g(f,hyperbox,'uniform',1e-5,0,'transform','C1sin')
q =
    0.2500
Example 2
% Estimate the integral with integrand f(x) = x1.^2.*x2.^2.*x3.^2
% in the interval R^3 where x1, x2 and x3 are normally distributed:
  f = Q(x) x(:,1).^2.*x(:,2).^2.*x(:,3).^2; \text{ hyperbox} = [-inf(1,3);inf(1,3)];
  q = cubLattice_g(f,hyperbox,'normal',1e-3,1e-3,'transform','C1sin')
q =
    1.0000
Example 3
% Estimate the integral with integrand f(x) = \exp(-x1^2-x2^2) in the
% interval [-1,2)^2:
```

 $f = @(x) \exp(-x(:,1).^2-x(:,2).^2); \text{ hyperbox} = [-ones(1,2); 2*ones(1,2)];$

q = cubLattice_g(f,hyperbox,'uniform',1e-3,1e-2,'transform','C1')

```
q =
    2.6532
Example 4
% Estimate the price of an European call with SO=100, K=100, r=sigma^2/2,
\% sigma=0.05 and T=1.
  f = @(x) \exp(-0.05^2/2)*max(100*exp(0.05*x)-100,0); hyperbox = [-inf(1,1);inf(1,1)];
  q = cubLattice_g(f,hyperbox,'normal',1e-4,1e-2,'fudge',@(m) 2.^-(2*m),'transform','C1sin')
q =
    2.0563
Example 5
% Estimate the integral with integrand f(x) = 8*x1.*x2.*x3.*x4.*x5 in the
% interval [0,1)^5 with pure absolute error 1e-5.
  f = Q(x)  8*prod(x,2); hyperbox = [zeros(1,5); ones(1,5)];
  q = cubLattice_g(f,hyperbox,'uniform',1e-5,0)
q =
    0.2500
Example 6
% Estimate the integral with integrand f(x) = 3./(5-4*(cos(2*pi*x))) in the interval
\% [0,1) with pure absolute error 1e-5.
  f = 0(x) 3./(5-4*(cos(2*pi*x))); hyperbox = [0;1];
  q = cubLattice_g(f,hyperbox,'uniform',1e-5,0,'transform','id')
q =
    1.0000
```

8.5 See Also

cubSobol_g, cubMC_g, meanMC_g, meanMCBer_g, integral_g

9 cubSobol_g

Quasi-Monte Carlo method using Sobol' cubature over the d-dimensional region to integrate within a specified generalized error tolerance with guarantees under Walsh-Fourier coefficients cone decay assumptions

9.1 Syntax

```
[q,out_param] = cubSobol_g(f,hyperbox)

q = cubSobol_g(f,hyperbox,measure,abstol,reltol)

q = cubSobol_g(f,hyperbox,'measure',measure,'abstol',abstol,'reltol',reltol)

q = cubSobol_g(f,hyperbox,in_param)
```

9.2 Description

[q,out_param] = $\operatorname{cubSobol_g}(f, \operatorname{hyperbox})$ estimates the integral of f over the d-dimensional region described by hyperbox, and with an error guaranteed not to be greater than a specific generalized error tolerance, tolfun:=max(abstol,reltol*| integral(f) |). Input f is a function handle. f should accept an n x d matrix input, where d is the dimension and n is the number of points being evaluated simultaneously. The input hyperbox is a 2 x d matrix, where the first row corresponds to the lower limits and the second row corresponds to the upper limits of the integral. Given the construction of Sobol' sequences, d must be a positive integer with 1 <= d <= 1111.

 $q = cubSobol_g(f,hyperbox,measure,abstol,reltol)$ estimates the integral of f over the hyperbox. The answer is given within the generalized error tolerance tolfun. All parameters should be input in the order specified above. If an input is not specified, the default value is used. Note that if an input is not specified, the remaining tail cannot be specified either. Inputs f and hyperbox are required. The other optional inputs are in the correct order: measure,abstol,reltol,mmin,mmax,fudge,toltype and theta.

q = **cubSobol_g**(f,hyperbox,'measure',measure,'abstol',abstol,'reltol',reltol) estimates the integral of f over the hyperbox. The answer is given within the generalized error tolerance tolfun. All the field-value pairs are optional and can be supplied in any order. If an input is not specified, the default value is used.

 $q = \mathbf{cubSobol_g}(f, hyperbox, in_param)$ estimates the integral of f over the hyperbox. The answer is given within the generalized error tolerance tolfun.

Input Arguments

- f the integrand whose input should be a matrix n x d where n is the number of data points and d the dimension, which cannot be greater than 1111. By default f is f=@ x.^2.
- hyperbox the integration region defined by its bounds. It must be a 2 x d matrix, where the first row corresponds to the lower limits and the second row corresponds to the upper limits of the integral. The default value is [0;1].
- in_param.measure for f(x)*mu(dx), we can define mu(dx) to be the measure of a uniformly distributed random variable in the hyperbox or normally distributed with covariance matrix I_d. The only possible values are 'uniform' or 'normal'. For 'uniform', the hyperbox must be a finite volume while for 'normal', the hyperbox can only be defined as (-Inf,Inf)^d. By default it is 'uniform'.
- in_param.abstol the absolute error tolerance, abstol>=0. By default it is 1e-4.
- in_param.reltol the relative error tolerance, which should be in [0,1]. Default value is 1e-2.

Optional Input Arguments

- in_param.mmin the minimum number of points to start is 2^mmin. The cone condition on the Fourier coefficients decay requires a minimum number of points to start. The advice is to consider at least mmin=10. mmin needs to be a positive integer with mmin<=mmax. By default it is 10.
- in_param.mmax the maximum budget is 2^mmax. By construction of the Sobol' generator, mmax is a positive integer such that mmin<=mmax<=53. The default value is 24.
- in_param.fudge the positive function multiplying the finite sum of Fast Walsh Fourier coefficients specified in the cone of functions. This input is a function handle. The fudge should accept an array of nonnegative integers being evaluated simultaneously. For more technical information about this parameter, refer to the references. By default it is @(m) 5*2.^-m.
- in-param.toltype this is the generalized tolerance function. There are two choices, 'max' which takes max(abstol,reltol*| integral(f) |) and 'comb' which is the linear combination theta*abstol+(1-theta)*reltol*| integral(f) | . Theta is another parameter to be specified with 'comb'(see below). For pure absolute error, either choose 'max' and set reltol = 0 or choose 'comb' and set theta = 1. For pure relative error, either choose 'max' and set abstol = 0 or choose 'comb' and set theta = 0. Note that with 'max', the user can not input abstol = reltol = 0 and with 'comb', if theta = 1 abstol con not be 0 while if theta = 0, reltol can not be 0. By default toltype is 'max'.
- in_param.theta this input is parametrizing the toltype 'comb'. Thus, it is only active when the toltype chosen is 'comb'. It establishes the linear combination weight between the absolute and relative tolerances theta*abstol+(1-theta)*reltol*| integral(f) |. Note that for theta = 1, we have pure absolute tolerance while for theta = 0, we have pure relative tolerance. By default, theta=1.

Output Arguments

- q the estimated value of the integral.
- out_param.d dimension over which the algorithm integrated.
- out_param.n number of Sobol' points used for comupting the integral of f.
- out_param.bound_err predicted bound on the error based on the cone condition. If the function lies in the cone, the real error will be smaller than generalized tolerance.
- out_param.time time elapsed in seconds when calling cubSobol_g.
- out_param.exitflag this is a binary vector stating whether warning flags arise. These flags tell about which conditions make the final result certainly not guaranteed. One flag is considered arisen when its value is 1. The following list explains the flags in the respective vector order:
 - 1 If reaching overbudget. It states whether the max budget is attained without reaching the guaranteed error tolerance.
 - 2 If the function lies outside the cone. In this case, results are not guaranteed. For more information about the cone definition, check the article mentioned below.

9.3 Guarantee

This algorithm computes the integral of real valued functions in dimension d with a prescribed generalized error tolerance. The Walsh-Fourier coefficients of the integrand are assumed to be absolutely convergent. If the algorithm terminates without warning messages, the output is given with guarantees under the assumption that the integrand lies inside a cone of functions. The guarantee is based on the decay rate of the Walsh-Fourier coefficients. For more details on how the cone is defined, please refer to the references below.

9.4 Examples

Example 1

```
% Estimate the integral with integrand f(x) = x1.*x2 in the interval
% [0,1)^2:
  f = Q(x) \operatorname{prod}(x,2); hyperbox = [zeros(1,2); ones(1,2)];
  q = cubSobol_g(f,hyperbox,'uniform',1e-5,0)
q =
    0.2500
Example 2
% Estimate the integral with integrand f(x) = x1.^2.*x2.^2.*x3.^2
% in the interval R^3 where x1, x2 and x3 are normally distributed:
  f = @(x) x(:,1).^2.*x(:,2).^2.*x(:,3).^2; \text{ hyperbox} = [-inf(1,3);inf(1,3)];
  q = cubSobol_g(f,hyperbox,'normal',1e-3,1e-3)
q =
    0.9998
Example 3
% Estimate the integral with integrand f(x) = \exp(-x1^2-x2^2) in the
% interval [-1,2)^2:
  f = @(x) \exp(-x(:,1).^2-x(:,2).^2); \text{ hyperbox} = [-ones(1,2); 2*ones(1,2)];
  q = cubSobol_g(f,hyperbox,'uniform',1e-3,1e-2)
q =
    2.6533
Example 4
% Estimate the price of an European call with SO=100, K=100, r=sigma^2/2,
% sigma=0.05 and T=1.
  f = @(x) \exp(-0.05^2/2)*max(100*exp(0.05*x)-100,0); hyperbox = [-inf(1,1);inf(1,1)];
  q = cubSobol_g(f,hyperbox,'normal',1e-4,1e-2,'fudge',0(m) 2.^-(2*m))
q =
    2.0586
```

Example 5

```
% Estimate the integral with integrand f(x) = 8*x1.*x2.*x3.*x4.*x5 in the
% interval [0,1)^5 with pure absolute error 1e-5.

f = @(x) 8*prod(x,2); hyperbox = [zeros(1,5);ones(1,5)];
q = cubSobol_g(f,hyperbox,'uniform',1e-5,0)

q =
    0.2500
```

9.5 See Also

 $cubLattice_g,\ cubMC_g,\ meanMC_g,\ meanMCBer_g,\ integral_g$

References

- [1] Jonathan B. Buckheit and David L. Donoho. Wavelab and reproducible research. Springer, 1995.
- [2] Sou-Cheng Choi, David L. Donoho, Ana Georgina Flesia, Xiaoming Huo, Ofer Levi, and Danzhu Shi. About Beamlab—a toolbox for new multiscale methodologies. Technical report, 2002.
- [3] Sou-Cheng T. Choi. MINRES-QLP Pack and reliable reproducible research via supportable scientific software. *Journal of Open Research Software*, 2(1), 2014.
- [4] Sou-Cheng T. Choi and Fred J. Hickernell. IIT MATH-573 Reliable Mathematical Software, 2013.
- [5] Sou-Cheng T. Choi, Fred J. Hickernell, Yuhan Ding, Lan Jiang, Lluís Antoni Jiménez Rugama, Xin Tong, Yizhi Zhang, and Xuan Zhou. GAIL: Guaranteed Automatic Integration Library (Version 2.1), MATLAB Software, 2015.
- [6] Jon Claerbout. Reproducible Computational Research: A history of hurdles, mostly overcome.
- [7] Nicholas Clancy, Yuhan Ding, Caleb Hamilton, Fred J. Hickernell, and Yizhi Zhang. The cost of deterministic, adaptive, automatic algorithms: Cones, not balls. *Journal of Complexity*, 30:21–45, 2014.
- [8] Yuhan Ding, Fred J. Hickernell, and Sou-Cheng T. Choi. Locally adaptive method for approximating univariate functions in cones with a guarantee for accuracy. Technical report, 2015. Working.
- [9] Fred J. Hickernell, Lan Jiang, Yuewei Liu, and Art B. Owen. In J. Dick, editor, *Monte Carlo and Quasi-Monte Carlo methods 2012*, pages 105–128. Springer-Verlag, Berlin.
- [10] Fred J. Hickernell and Lluís Antoni Jiménez Rugama. Reliable adaptive cubature using digital sequences. Technical report, 2014. Submitted.
- [11] Lan Jiang and Fred J. Hickernell. Guaranteed conservative confidence intervals for means of Bernoulli random variables. Technical report, 2014. Submitted.
- [12] Daniel Katz, Sou-Cheng Choi, Hilmar Lapp, Ketan Maheshwari, Frank Löffler, Matthew Turk, Marcus Hanwell, Nancy Wilkins-Diehr, James Hetherington, James Howison, Shel Swenson, Gabrielle Allen, Anne Elster, Bruce Berriman, and Colin Venters. Summary of the first workshop on sustainable software for science: Practice and experiences (WSSSPE1). Journal of Open Research Software, 2(1), 2014.
- [13] Lluís Antoni Jiménez Rugama and Fred J. Hickernell. Adaptive multidimensional integration based on rank-1 lattices. Technical report, 2014. Submitted.
- [14] Xin Tong. A guaranteed, adaptive, automatic algorithm for univariate function minimization, 2014. MS Thesis.