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# Guaranteed Automatic Integration Library (GAIL) 2.1 User Guide

GAIL (Guaranteed Automatic Integration Library) is created, developed, and maintained by Fred Hickernell (Illinois Institute of Technology), Sou-Cheng Choi (NORC at the University of Chicago and IIT), Yuhang Ding (IIT), Lan Jiang (IIT), Lluís Antoni Jimenez Rugama (IIT), Xin Tong (University of Illinois at Chicago), Yizhi Zhang (IIT), and Xuan Zhou (IIT).

GAIL is a suite of algorithms for integration problems in one, many, and infinite dimensions, and whose answers are guaranteed to be correct.

`%help GAU`

## Functions

## Installation

## 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)**;

To run all the fast doctests and unit tests in the suite, execute the script **runtests.m**.

A collection of long tests are contained in **longtests.m**.

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# Website

For more information about GAIL, visit [Gailteam](#)

## Functions

### 1-D approximation

### 1-D integration

### High dimension integration

### 1-D minimization

## funappx\_g

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

## 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,...)`

## Description

`fappx = funappx_g(f)` approximates function  $f$  on the default interval  $[0,1]$  by an approximated function `fappx` within the guaranteed absolute error tolerance of  $1e-6$ . 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',a,'b',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.

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$f_{\text{appx}} = \text{funappx\_g}(f, \text{in\_param})$  approximates function  $f$  on the finite interval  $[\text{in\_param.a}, \text{in\_param.b}]$ , given a guaranteed absolute error tolerance  $\text{in\_param.abstol}$ . If a field is not specified, the default value is used.

$[\text{fappx}, \text{out\_param}] = \text{funappx\_g}(f, \dots)$  returns an approximated function  $\text{fappx}$  and an output structure  $\text{out\_param}$ .

### Input Arguments

- $f$  --- input function
- $\text{in\_param.a}$  --- left end point of interval, default value is 0
- $\text{in\_param.b}$  --- right end point of interval, default value is 1
- $\text{in\_param.abstol}$  --- guaranteed absolute error tolerance, default value is  $1e-6$

### Optional Input Arguments

- $\text{in\_param.nlo}$  --- lower bound of initial number of points we used, default value is 10
- $\text{in\_param.nhi}$  --- upper bound of initial number of points we used, default value is 1000
- $\text{in\_param.nmax}$  --- when number of points hits the value, iteration will stop, default value is  $1e7$
- $\text{in\_param.maxiter}$  --- max number of iterations, default value is 1000

### Output Arguments

- $\text{fappx}$  --- approximated function
- $\text{out\_param.f}$  --- input function
- $\text{out\_param.a}$  --- left end point of interval
- $\text{out\_param.b}$  --- right end point of interval
- $\text{out\_param.abstol}$  --- guaranteed absolute error tolerance
- $\text{out\_param.nlo}$  --- a lower bound of initial number of points we use
- $\text{out\_param.nhi}$  --- an upper bound of initial number of points we use
- $\text{out\_param.nmax}$  --- when number of points hits the value, iteration will stop
- $\text{out\_param.maxiter}$  --- max number of iterations
- $\text{out\_param.ninit}$  --- initial number of points we use for each sub interval
- $\text{out\_param.exit}$  --- this is a number defining the conditions of success or failure satisfied when finishing the algorithm. The algorithm is considered successful (with  $\text{out\_param.exit} == 0$ ) 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

## 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

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

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

$$\|f - f_{appx}\|_{\infty} \leq abstol$$

## Examples

### 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.
```

```
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]

```

### 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 = @(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]
```

## See Also

## References

- [1] Nick 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 (2014), pp. 21-45.
- [2] Yuhan Ding, Fred J. Hickernell, and Sou-Cheng T. Choi, "Locally Adaptive Method for Approximating Univariate Functions in Cones with a Guarantee for Accuracy", working, 2015.
- [3] Sou-Cheng T. Choi, Yuhan Ding, Fred J. Hickernell, Lan Jiang, Lluís Antoni Jimenez Rugama, Xin Tong, Yizhi Zhang and Xuan Zhou, "GAIL: Guaranteed Automatic Integration Library (Version 2.1)" [MATLAB Software], 2015. Available from <http://code.google.com/p/gail/>
- [4] Sou-Cheng T. Choi, "MINRES-QLP Pack and Reliable Reproducible Research via Supportable Scientific Software", *Journal of Open Research Software*, Volume 2, Number 1, e22, pp. 1-7, DOI: <http://dx.doi.org/10.5334/jors.bb>, 2014.
- [5] Sou-Cheng T. Choi and Fred J. Hickernell, "IIT MATH-573 Reliable Mathematical Software" [Course Slides], Illinois Institute of Technology, Chicago, IL, 2013. Available from <http://code.google.com/p/gail/>
- [6] Sou-Cheng T. Choi, "Summary of the First Workshop On Sustainable Software for Science: Practice And Experiences (WSSSPE1)", *Journal of Open Research Software*, Volume 2, Number 1, e6, pp. 1-21, DOI: <http://dx.doi.org/10.5334/jors.an>, 2014.

If you find GAIL helpful in your work, please support us by citing the above papers, software, and materials.

## funmin\_g

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



---

# Syntax

```
fmin = funmin_g(f)

fmin = funmin_g(f,a,b,abstol,TolX)

fmin = funmin_g(f,'a','b','abstol',abstol,'TolX',TolX)

fmin = funmin_g(f,in_param)

[fmin, out_param] = funmin_g(f,...)
```

## 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','abstol',abstol,'TolX',TolX)` finds minimum value of function `f` on the interval `[a,b]` with a guaranteed absolute error tolerance `abstol` and a guaranteed X tolerance `TolX`. All five field-value pairs are optional and can be supplied in different order.

`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.

## Guarantee

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

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

then the `fmin` output by this algorithm is guaranteed to satisfy

$$|\min f - f_{\min}| \leq \text{abstol}$$

or

$$\mathrm{volumeX} \leq \mathrm{TolX},$$

provided the flag `exitflag=0`.

## Examples

### Example 1

```
f=@(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  
    rmax: 10000000  
   ninit: 100  
    tau: 197  
exitflag: 0  
  npoints: 6337  
   errest: 6.1554e-07  
  volumeX: 0.0015  
tauchange: 0  
intervals: [2x1 double]
```

## Example 2

```
f=@(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  
    rmax: 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=@(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]
```

## See Also

## References

- [1] Xin Tong. A Guaranteed, Adaptive, Automatic Algorithm for Univariate Function Minimization. MS thesis, Illinois Institute of Technology, 2014.
- [2] Sou-Cheng T. Choi, Yuhang Ding, Fred J. Hickernell, Lan Jiang, Lluís Antoni Jiménez Rugama, Xin Tong, Yizhi Zhang and Xuan Zhou, "GAIL: Guaranteed Automatic Integration Library (Version 2.1)" [MATLAB Software], 2015. Available from <http://code.google.com/p/gail/>
- [3] Sou-Cheng T. Choi, "MINRES-QLP Pack and Reliable Reproducible Research via Supportable Scientific Software", Journal of Open Research Software, Volume 2, Number 1, e22, pp. 1-7, DOI: <http://dx.doi.org/10.5334/jors.bb>, 2014.
- [4] Sou-Cheng T. Choi and Fred J. Hickernell, "IIT MATH-573 Reliable Mathematical Software" [Course Slides], Illinois Institute of Technology, Chicago, IL, 2013. Available from <http://code.google.com/p/gail/>
- [5] Sou-Cheng T. Choi, "Summary of the First Workshop On Sustainable Software for Science: Practice And Experiences (WSSSPE1)", Journal of Open Research Software, Volume 2, Number 1, e6, pp. 1-21, DOI: <http://dx.doi.org/10.5334/jors.an>, 2014.

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---

# integral\_g

1-D guaranteed function integration using trapezoidal rule

## 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,...)
```

## 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
- `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`

## Guarantee

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

$$\|f''\|_1 \leq \frac{nstar}{2(b-a)} \left\| f' - \frac{f(b) - f(a)}{b-a} \right\|_1,$$

then the  $q$  output by this algorithm is guaranteed to satisfy

$$\left\| \int_a^b f(x) dx - q \right\| \leq abstol$$

provided the flag `exceedbudget= 0`.

---

And the upper bound of the cost is

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

## Examples

### Example 1

```
f = @(x) x.^2; [q, out_param] = integral_g(f)

% Integrate function x with default input parameter to make the error less
% 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
    ninit: 100
    tau: 197
    exceedbudget: 0
    tauchange: 0
    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 toerence 1e-8

q =

    0.1353

out_param =

    a: 1
```



---

```
abstol: 1.0000e-05
      b: 2
      f: @(x)exp(-x.^2)
      nhi: 10000
      nlo: 100
      nmax: 10000000
      ninit: 1000
      tau: 1997
exceedbudget: 0
tauchange: 0
npoints: 2998
errest: 7.3718e-06
```

## See Also

## References

- [1] Nick 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 (2014), pp. 21-45.
- [2] Sou-Cheng T. Choi, Yuhan Ding, Fred J. Hickernell, Lan Jiang, Lluís Antoni Jimenez Rugama, Xin Tong, Yizhi Zhang and Xuan Zhou, "GAIL: Guaranteed Automatic Integration Library (Version 2.1)" [MATLAB Software], 2015. Available from <http://code.google.com/p/gail/>
- [3] Sou-Cheng T. Choi, "MINRES-QLP Pack and Reliable Reproducible Research via Supportable Scientific Software", *Journal of Open Research Software*, Volume 2, Number 1, e22, pp. 1-7, DOI: <http://dx.doi.org/10.5334/jors.bb>, 2014.
- [4] Sou-Cheng T. Choi and Fred J. Hickernell, "IIT MATH-573 Reliable Mathematical Software" [Course Slides], Illinois Institute of Technology, Chicago, IL, 2013. Available from <http://code.google.com/p/gail/>
- [5] Sou-Cheng T. Choi, "Summary of the First Workshop On Sustainable Software for Science: Practice And Experiences (WSSSPE1)", *Journal of Open Research Software*, Volume 2, Number 1, e6, pp. 1-21, DOI: <http://dx.doi.org/10.5334/jors.an>, 2014.

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## meanMC\_g

MEANMC\_G Monte Carlo method to estimate the mean of a random variable.

## Syntax

```
tmu = meanMC_g(Yrand)
```

```
tmu = meanMC_g(Yrand,abstol,reltol,alpha)
```

```
tmu = meanMC_g(Yrand,'abstol',abstol,'reltol',reltol,'alpha',alpha)
```

---

[tmu, out\_param] = **meanMC\_g**(Yrand,in\_param)

## Description

tmu = **meanMC\_g**(Yrand) estimates the mean,  $\mu$ , of a random variable  $Y$  to within a specified generalized error tolerance,  $\text{tolfun} := \max(\text{abstol}, \text{reltol} * |\mu|)$ , i.e.,  $\mu - \text{tmu} \leq \text{tolfun}$  with probability at least  $1 - \alpha$ , where  $\text{abstol}$  is the absolute error tolerance, and  $\text{reltol}$  is the relative error tolerance. Usually the  $\text{reltol}$  determines the accuracy of the estimation, however, if the  $\mu$  is rather small, the  $\text{abstol}$  determines the accuracy of the estimation. The default values are  $\text{abstol} = 1e-2$ ,  $\text{reltol} = 1e-1$ , and  $\alpha = 1\%$ . Input  $Yrand$  is a function handle that accepts a positive integer input  $n$  and returns an  $n \times 1$  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  $\text{tolfun}$  with guaranteed confidence level  $1 - \alpha$  using all ordered parsing inputs  $\text{abstol}$ ,  $\text{reltol}$ ,  $\alpha$ .

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  $\text{tolfun}$  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  $\text{tolfun}$  with the given parameters  $\text{in\_param}$  and produce the estimated mean  $\text{tmu}$  and output parameters  $\text{out\_param}$ . 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  $Yrand = @(n) \text{rand}(n,1).^2$ .
- $\text{in\_param.abstol}$  --- the absolute error tolerance, which should be positive, default value is  $1e-2$ .
- $\text{in\_param.reltol}$  --- the relative error tolerance, which should be between 0 and 1, default value is  $1e-1$ .
- $\text{in\_param.alpha}$  --- the uncertainty, which should be a small positive percentage. default value is  $1\%$ .

### Optional Input Arguments

- $\text{in\_param.fudge}$  --- standard deviation inflation factor, which should be larger than 1, default value is 1.2.
- $\text{in\_param.nSig}$  --- initial sample size for estimating the sample variance, which should be a moderate large integer at least 30, the default value is  $1e4$ .
- $\text{in\_param.n1}$  --- initial sample size for estimating the sample mean, which should be a moderate large positive integer at least 30, the default value is  $1e4$ .
- $\text{in\_param.tbudget}$  --- the time budget in seconds to do the two-stage estimation, which should be positive, the default value is 100 seconds.
- $\text{in\_param.nbudget}$  --- 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`

## Guarantee

This algorithm attempts to calculate the mean,  $\mu$ , of a random variable to a prescribed error tolerance, `tolfun:= max(abstol,reltol*|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:

$$\Pr(\mu - \text{tmu} \leq \text{tolfun}) \geq 1 - \alpha$$

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

$$\Pr(N_{\text{tot}} \leq N_{\text{up}}) \geq 1 - \beta$$

Please refer to our paper for detailed arguments and proofs.

## Examples

### Example 1

```
% Calculate the mean of x^2 when x is uniformly distributed in
% [0 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=@(n) rand(n,1).^2;
tmu = meanMC_g(Yrand,in_param)
```

---

```
tmu =  
  
0.3332
```

### Example 2

```
% Calculate the mean of exp(x) when x is uniformly distributed in  
% [0 1], with the absolute error tolerance 1e-3.
```

```
tmu = meanMC_g(@(n)exp(rand(n,1)),1e-3,0)
```

```
tmu =  
  
1.7182
```

### 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 =  
  
0.8421
```

## See Also

## References

- [1] F. J. Hickernell, L. Jiang, Y. Liu, and A. B. Owen, Guaranteed conservative fixed width confidence intervals via Monte Carlo sampling, Monte Carlo and Quasi-Monte Carlo Methods 2012 (J. Dick, F. Y. Kuo, G. W. Peters, and I. H. Sloan, eds.), Springer-Verlag, Berlin, 2014. arXiv:1208.4318 [math.ST]
- [2] Sou-Cheng T. Choi, Yuhang Ding, Fred J. Hickernell, Lan Jiang, Lluís Antoni Jimenez Rugama, Xin Tong, Yizhi Zhang and Xuan Zhou, "GAIL: Guaranteed Automatic Integration Library (Version 2.1)" [MATLAB Software], 2015. Available from <http://code.google.com/p/gail/>
- [3] Sou-Cheng T. Choi, "MINRES-QLP Pack and Reliable Reproducible Research via Supportable Scientific Software", Journal of Open Research Software, Volume 2, Number 1, e22, pp. 1-7, DOI: <http://dx.doi.org/10.5334/jors.bb>, 2014.
- [4] Sou-Cheng T. Choi and Fred J. Hickernell, "IIT MATH-573 Reliable Mathematical Software" [Course Slides], Illinois Institute of Technology, Chicago, IL, 2013. Available from <http://code.google.com/p/gail/>

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## 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  $1-\alpha$ .

## 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)
```

## 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  $n \times 1$  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.

## Guarantee

If the sample size is calculated according Hoeffding's inequality, which equals to  $\text{ceil}(\log(2/\text{out\_param.alpha})/(2*\text{out\_param.abstol}^2))$ , then the following inequality must be satisfied:

$$\Pr(p - \text{pHat} \leq \text{abstol}) \geq 1 - \alpha.$$

Here  $p$  is the true mean of `Yrand`, and `pHat` is the output of `MEANMCBER_G`

Also, the cost is deterministic.

## 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;
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 =
```

## See Also

## References

- [1] F. J. Hickernell, L. Jiang, Y. Liu, and A. B. Owen, Guaranteed conservative fixed width confidence intervals via Monte Carlo sampling, Monte Carlo and Quasi-Monte Carlo Methods 2012 (J. Dick, F. Y. Kuo, G. W. Peters, and I. H. Sloan, eds.), Springer-Verlag, Berlin, 2014. arXiv:1208.4318 [math.ST]
- [2] Sou-Cheng T. Choi, Yuhang Ding, Fred J. Hickernell, Lan Jiang, Lluís Antoni Jimenez Rugama, Xin Tong, Yizhi Zhang and Xuan Zhou, "GAIL: Guaranteed Automatic Integration Library (Version 2.1)" [MATLAB Software], 2015. Available from <http://code.google.com/p/gail/>
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## cubMC\_g

Monte Carlo method to evaluate a multidimensional integral

## Syntax

```
[Q,out_param] = cubMC_g(f,hyperbox)
Q = cubMC_g(f,hyperbox,measure,abstol,reltol,alpha)
Q = cubMC_g(f,hyperbox,'measure',measure,'abstol',abstol,'reltol',reltol,'alpha',alpha)
[Q out_param] = cubMC_g(f,hyperbox,in_param)
```

## Description

`[Q,out_param] = cubMC_g(f,hyperbox)` estimates the integral of  $f$  over hyperbox to within a specified generalized error tolerance,  $\text{tolfun} = \max(\text{abstol}, \text{reltol} * |I|)$ , i.e.,  $|I - Q| \leq \text{tolfun}$  with probability at least  $1 - \alpha$ , where  $\text{abstol}$  is the absolute error tolerance, and  $\text{reltol}$  is the relative error tolerance. Usually the

---

reitol 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, reitol=1e-1, and alpha=1%. Input f is a function handle that accepts an  $n \times d$  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  $2 \times d$  matrix, where the first row corresponds to the lower limits and the second row corresponds to the upper limits.

$Q = \text{cubMC\_g}(f, \text{hyperbox}, \text{measure}, \text{abstol}, \text{reitol}, \text{alpha})$  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, reitol, alpha, fudge, nSig, n1, tbudget, nbudget, flag. The input f and hyperbox are required and others are optional.

$Q = \text{cubMC\_g}(f, \text{hyperbox}, \text{'measure'}, \text{measure}, \text{'abstol'}, \text{abstol}, \text{'reitol'}, \text{reitol}, \text{'alpha'}, \text{alpha})$  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.

$[Q \text{ out\_param}] = \text{cubMC\_g}(f, \text{hyperbox}, \text{in\_param})$  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  $[\text{zeros}(1,d); \text{ones}(1,d)]$ , 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.reitol --- 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.
  - `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'

```

## Guarantee

This algorithm attempts to calculate the integral of function  $f$  over a hyperbox to a prescribed error tolerance  $\text{tolfun} := \max(\text{abstol}, \text{reltol} * |I|)$  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:

$$\Pr(Q - I \leq \text{tolfun}) \geq 1 - \alpha$$

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

$$\Pr(N_{\text{tot}} \leq N_{\text{up}}) \geq 1 - \beta$$

Please refer to our paper for detailed arguments and proofs.

## Examples

### Example 1

---

```
% Estimate the integral with integrand f(x) = sin(x) over the interval
% [1;2]
%
```

```
f=@(x) sin(x);interval = [1;2];
Q = cubMC_g(f,interval,'uniform',1e-3,1e-2)
```

$Q =$

0.9565

### 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 = @(x) exp(-x(:,1).^2-x(:,2).^2); hyperbox = [0 0;1 1];
Q = cubMC_g(f,hyperbox,'measure','uniform','abstol',1e-3,...
    'reltol',1e-13)
```

$Q =$

0.5578

### 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=@(x) 2^d*prod(x,2)+0.555; hyperbox =[zeros(1,d);ones(1,d)];
in_param.abstol = 1e-3;in_param.reltol=1e-3;
Q = cubMC_g(f,hyperbox,in_param)
```

$Q =$

1.5554

### 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 =  
  
0.3329
```

## See Also

## References

- [1] F. J. Hickernell, L. Jiang, Y. Liu, and A. B. Owen, Guaranteed conservative fixed width confidence intervals via Monte Carlo sampling, Monte Carlo and Quasi-Monte Carlo Methods 2012 (J. Dick, F. Y. Kuo, G. W. Peters, and I. H. Sloan, eds.), pp. 105-128, Springer-Verlag, Berlin, 2014 DOI: 10.1007/978-3-642-41095-6\_5
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- [5] Sou-Cheng T. Choi, "Summary of the First Workshop On Sustainable Software for Science: Practice And Experiences (WSSSPE1)", Journal of Open Research Software, Volume 2, Number 1, e6, pp. 1-21, DOI: <http://dx.doi.org/10.5334/jors.an>, 2014.

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## 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.

## Syntax

```
[q,out_param] = cubLattice_g(f,d)  
  
q = cubLattice_g(f,d,abstol,reltol,measure,shift,mmin,mmax,fudge,transform,toltype,theta)
```

---

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

## Description

`[q,out_param] = cubLattice_g(f,d)` estimates the integral of  $f$  over the  $d$ -dimensional region with an error guaranteed not to be greater than a specific generalized error tolerance,  $\text{tolfun} := \max(\text{abstol}, \text{reitol} * \text{abs}(\text{integral}(f)))$ . The generalized tolerance function can also be chosen as  $\text{tolfun} := \theta * \text{abstol} + (1 - \theta) * \text{reitol} * \text{abs}(\text{integral}(f))$  where  $\theta$  is another input parameter. Input  $f$  is a function handle.  $f$  should accept an  $n \times d$  matrix input, where  $d$  is the dimension of the hypercube, and  $n$  is the number of points being evaluated simultaneously. The input  $d$  is the dimension in which the function  $f$  is defined. Given the construction of our Lattices,  $d$  must be a positive integer with  $1 \leq d \leq 250$ .

`q = cubLattice_g(f,d,abstol,reitol,measure,shift,mmin,mmax,fudge,transform,toltype,theta)` estimates the integral of  $f$  over a  $d$ -dimensional region. The answer is given within the generalized error tolerance  $\text{tolfun}$ . 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.

`q = cubLattice_g(f,d,in_param)` estimates the integral of  $f$  over the  $d$ -dimensional region. The answer is given within the generalized error tolerance  $\text{tolfun}$ .

### Input Arguments

- $f$  --- the integrand whose input should be a matrix  $n \times d$  where  $n$  is the number of data points and  $d$  the dimension. By default it is the quadratic function.
- $d$  --- dimension of domain on which  $f$  is defined.  $d$  must be a positive integer  $1 \leq d \leq 250$ . By default it is 1.
- `in_param.abstol` --- the absolute error tolerance,  $\text{abstol} > 0$ . By default it is  $1e-4$ .
- `in_param.reitol` --- the relative error tolerance, which should be in  $[0,1]$ . Default value is  $1e-1$ .
- `in_param.measure` --- for  $f(x) * \mu(dx)$ , we can define  $\mu(dx)$  to be the measure of a uniformly distributed random variable in  $[0,1]^d$  or normally distributed with covariance matrix  $I_d$ . By default it is 'uniform'. The only possible values are 'uniform' or 'normal'.

### 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  $mmin \leq mmax$ . 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  $mmin \leq mmax \leq 26$ . 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. For more information about this parameter, refer to the references. By default it is  $@(x) 5 * 2.^{-x}$ .
- `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 Baker. The options: 'id' : no transformation. Choice by default. 'Baker': Baker's transform or tent map

---

in each coordinate. Preserving only continuity but simple to compute. 'C0': polynomial transformation only preserving continuity. 'C1': polynomial transformation preserving the first derivative. 'C1sin': Sidi transform with sinus preserving the first derivative. This is in general a better option than 'C1'.

- `in_param.toltype` --- this is the tolerance function. There are two choices, 'max' (chosen by default) which takes  $\max(\text{abstol}, \text{reltol} * |\text{integral}(f)|)$  and 'comb' which is a linear combination  $\text{theta} * \text{abstol} + (1 - \text{theta}) * \text{reltol} * |\text{integral}(f)|$ . Theta is another parameter that can be specified (see below). For pure absolute error, either choose 'max' and set `reltol=0` or choose 'comb' and set `theta=1`.
- `in_param.theta` --- this input is parametrizing the `toltype` 'comb'. Thus, it is only affecting when the `toltype` chosen is 'comb'. It establishes the linear combination weight between the absolute and relative tolerances  $\text{theta} * \text{abstol} + (1 - \text{theta}) * \text{reltol} * |\text{integral}(f)|$ . 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.n` --- number of points used when calling `cubLattice_g` for `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 should be smaller than this predicted error.
- `out_param.time` --- time elapsed in seconds when calling `cubLattice_g` for `f`.
- `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.
%
```

## 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.

## Examples

### Example 1

---

```
% Estimate the integral with integrand f(x) = x1.*x2 in the interval  
% [0,1)^2:
```

```
f = @(x) prod(x,2); d = 2;  
q = cubLattice_g(f,d,1e-5,1e-1,'uniform','transform','Clsin')
```

$q =$

0.2500

### Example 2

```
% Estimate the integral with integrand f(x) = x1.^2.*x2.^2.*x3.^2+0.11  
% in the interval R^3 where x1, x2 and x3 are normally distributed:
```

```
f = @(x) x(:,1).^2.*x(:,2).^2.*x(:,3).^2+0.11; d = 3;  
q = cubLattice_g(f,d,1e-3,1e-3,'normal','transform','Clsin')
```

$q =$

1.1100

### Example 3

```
% Estimate the integral with integrand f(x) = exp(-x1^2-x2^2) in the  
% interval [0,1)^2:
```

```
f = @(x) exp(-x(:,1).^2-x(:,2).^2); d = 2;  
q = cubLattice_g(f,d,1e-3,1e-1,'uniform','transform','C1')
```

$q =$

0.5577

### Example 4

```
% Estimate the price of an European call with S0=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); d = 1;  
q = cubLattice_g(f,d,1e-4,1e-1,'normal','fudge',@(m) 2.^-(2*m),...  
    'transform','Clsin')
```

$q =$

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 = @(x) 8*prod(x,2); d = 5;
q = cubLattice_g(f,d,1e-5,0)
```

$q =$

*0.2500*

## See Also

## References

[1] Lluís Antoni Jimenez Rugama and Fred J. Hickernell: Adaptive Multidimensional Integration Based on Rank-1 Lattices (2014). Submitted for publication: arXiv:1411.1966.

[2] Sou-Cheng T. Choi, Fred J. Hickernell, Yuhang Ding, Lan Jiang, Lluís Antoni Jimenez Rugama, Xin Tong, Yizhi Zhang and Xuan Zhou, "GAIL: Guaranteed Automatic Integration Library (Version 2.1)" [MATLAB Software], 2015. Available from <http://code.google.com/p/gail/>

[3] Sou-Cheng T. Choi, "MINRES-QLP Pack and Reliable Reproducible Research via Supportable Scientific Software", Journal of Open Research Software, Volume 2, Number 1, e22, pp. 1-7, DOI: <http://dx.doi.org/10.5334/jors.bb>, 2014.

[4] Sou-Cheng T. Choi and Fred J. Hickernell, "IIT MATH-573 Reliable Mathematical Software" [Course Slides], Illinois Institute of Technology, Chicago, IL, 2013. Available from <http://code.google.com/p/gail/>

[5] Sou-Cheng T. Choi, "Summary of the First Workshop On Sustainable Software for Science: Practice And Experiences (WSSSPE1)", Journal of Open Research Software, Volume 2, Number 1, e6, pp. 1-21, DOI: <http://dx.doi.org/10.5334/jors.an>, 2014.

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## 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

## Syntax

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

```
q = cubSobol_g(f,d,abstol,reltol,measure,mmin,mmax,fudge,thetype,theta)
```

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

---

# Description

$[q, out\_param] = \text{cubSobol\_g}(f, d)$  estimates the integral of  $f$  over the  $d$ -dimensional region with an error guaranteed not to be greater than a specific generalized error tolerance,  $tolfun := \max(abstol, reltol * \text{abs}(\text{integral}(f)))$ . The generalized tolerance function can also be chosen as  $tolfun := \theta * abstol + (1 - \theta) * reltol * \text{abs}(\text{integral}(f))$  where  $\theta$  is another input parameter. Input  $f$  is a function handle.  $f$  should accept an  $n \times d$  matrix input, where  $d$  is the dimension of the hypercube, and  $n$  is the number of points being evaluated simultaneously. The input  $d$  is the dimension in which the function  $f$  is defined. Given the construction of Sobol',  $d$  must be a positive integer with  $1 \leq d \leq 1111$ .

$q = \text{cubSobol\_g}(f, d, abstol, reltol, measure, mmin, mmax, fudge, tolttype, \theta)$  estimates the integral of  $f$  over a  $d$ -dimensional region. 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.

$q = \text{cubSobol\_g}(f, d, in\_param)$  estimates the integral of  $f$  over the  $d$ -dimensional region. The answer is given within the generalized error tolerance  $tolfun$ .

## Input Arguments

- $f$  --- the integrand whose input should be a matrix  $n \times d$  where  $n$  is the number of data points and  $d$  the dimension. By default it is the quadratic function.
- $d$  --- dimension of domain on which  $f$  is defined.  $d$  must be a positive integer  $1 \leq d \leq 1111$ . By default it is 1.
- $in\_param.abstol$  --- 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  $1e-1$ .
- $in\_param.measure$  --- for  $f(x) * \mu(dx)$ , we can define  $\mu(dx)$  to be the measure of a uniformly distributed random variable in  $[0, 1]^d$  or normally distributed with covariance matrix  $I_d$ . By default it is 'uniform'. The only possible values are 'uniform' or 'normal'.

## 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  $mmin \leq mmax$ . 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  $mmin \leq mmax \leq 53$ . The default value is 24.
- $in\_param.fudge$  --- the positive function multiplying the finite sum of Fast Walsh coefficients specified in the cone of functions. For more information about this parameter, refer to the references. By default it is  $@(x) 5^{2.^{-x}}$ .
- $in\_param.tolttype$  --- this is the tolerance function. There are two choices, 'max' (chosen by default) which takes  $\max(abstol, reltol * |\text{integral}(f)|)$  and 'comb' which is a linear combination  $\theta * abstol + (1 - \theta) * reltol * |\text{integral}(f)|$ .  $\theta$  is another parameter that can be specified (see below). For pure absolute error, either choose 'max' and set  $reltol=0$  or choose 'comb' and set  $\theta=1$ .
- $in\_param.\theta$  --- this input is parametrizing the  $tolttype$  'comb'. Thus, it is only affecting when the  $tolttype$  chosen is 'comb'. It establishes the linear combination weight between the absolute and relative tolerances  $\theta * abstol + (1 - \theta) * reltol * |\text{integral}(f)|$ . 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.n` --- number of points used when calling `cubSobol_g` for `f`.
- `out_param.pred_err` --- predicted bound on the error based on the cone condition. If the function lies in the cone, the real error should be smaller than this predicted error.
- `out_param.time` --- time elapsed in seconds when calling `cubSobol_g` for `f`.
- `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.
```

## 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.

## Examples

### Example 1

```
% Estimate the integral with integrand  $f(x) = x_1 \cdot x_2$  in the interval
%  $[0,1]^2$ :
```

```
f = @(x) x(:,1).*x(:,2); d = 2;
q = cubSobol_g(f,d,1e-5,1e-1,'uniform')
```

$q =$

*0.2500*

---

### Example 2

```
% Estimate the integral with integrand  $f(x) = x_1.^2.*x_2.^2.*x_3.^2+0.11$   
% in the interval  $R^3$  where  $x_1$ ,  $x_2$  and  $x_3$  are normally distributed:
```

```
f = @(x) x(:,1).^2.*x(:,2).^2.*x(:,3).^2+0.11; d = 3;  
q = cubSobol_g(f,d,1e-3,1e-3,'normal')
```

$q =$

1.1116

### Example 3

```
% Estimate the integral with integrand  $f(x) = \exp(-x_1^2-x_2^2)$  in the  
% interval  $[0,1]^2$ :
```

```
f = @(x) exp(-x(:,1).^2-x(:,2).^2); d = 2;  
q = cubSobol_g(f,d,1e-3,1e-1,'uniform')
```

$q =$

0.5577

### Example 4

```
% Estimate the price of an European call with  $S_0=100$ ,  $K=100$ ,  $r=\sigma^2/2$ ,  
%  $\sigma=0.05$  and  $T=1$ .
```

```
f = @(x) exp(-0.05^2/2)*max(100*exp(0.05*x)-100,0); d = 1;  
q = cubSobol_g(f,d,1e-4,1e-1,'normal','fudge',@(m) 2.^-(2*m))
```

$q =$

2.0573

### Example 5

```
% Estimate the integral with integrand  $f(x) = 8*x_1.*x_2.*x_3.*x_4.*x_5$  in the  
% interval  $[0,1]^5$  with pure absolute error  $1e-5$ .
```

```
f = @(x) 8*prod(x,2); d = 5;  
q = cubSobol_g(f,d,1e-5,0)
```

$q =$

0.2500

---

## See Also

## References

- [1] Fred J. Hickernell and Lluís Antoni Jimenez Rugama: Reliable adaptive cubature using digital sequences (2014). Submitted for publication: arXiv:1410.8615.
- [2] Sou-Cheng T. Choi, Fred J. Hickernell, Yuhang Ding, Lan Jiang, Lluís Antoni Jimenez Rugama, Xin Tong, Yizhi Zhang and Xuan Zhou, "GAIL: Guaranteed Automatic Integration Library (Version 2.1)" [MATLAB Software], 2015. Available from <http://code.google.com/p/gail/>
- [3] Sou-Cheng T. Choi, "MINRES-QLP Pack and Reliable Reproducible Research via Supportable Scientific Software", Journal of Open Research Software, Volume 2, Number 1, e22, pp. 1-7, DOI: <http://dx.doi.org/10.5334/jors.bb>, 2014.
- [4] Sou-Cheng T. Choi and Fred J. Hickernell, "IIT MATH-573 Reliable Mathematical Software" [Course Slides], Illinois Institute of Technology, Chicago, IL, 2013. Available from <http://code.google.com/p/gail/>
- [5] Sou-Cheng T. Choi, "Summary of the First Workshop On Sustainable Software for Science: Practice And Experiences (WSSSPE1)", Journal of Open Research Software, Volume 2, Number 1, e6, pp. 1-21, DOI: <http://dx.doi.org/10.5334/jors.an>, 2014.

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## Installation Instructions

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 or reinstall GAIL, execute **GAIL\_Uninstall**. To reinstall GAIL, execute **GAIL\_Install**.

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