

Package ‘SimplicialCubature’

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Title Integration of Functions Over Simplices

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Description Provides methods to integrate functions over m-dimensional simplices in n-dimensional Euclidean space. There are exact methods for polynomials and adaptive methods for integrating an arbitrary function.

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SimplicialCubature-package

Numerical integration of functions over simplices

Description

Provides methods to evaluate integrals of the form

$$\int_S f(x)dx,$$

where S is a simplex (or a union of simplices) in n -space and $f(x)$ is a function defined on S . The function $f(x)$ may be vector valued and the simplices can be m -dimensional simplices, $1 \leq m \leq n$. For example, if $m=n-1$, the package will evaluate a surface area integral; if $m=1$, the package will evaluate a line integral.

There are exact methods for polynomials and adaptive methods for integrating an arbitrary function. The two main functions are:

`adaptIntegrateSimplex` - integrate a general (possibly vector valued) function over a simplex using the method of Genz and Cools. It is expected that these methods will yield several significant digits, but not many digits of precision.

`integrateSimplexPolynomial` - integrate a single polynomial exactly over a simplex using either the Grundmann-Moller method or the Lasserre-Avrachenkov method.

The naming of the functions, arguments, and return values deliberately mimics that in the CRAN packages `cubature` (for integrating over hyper-rectangles) and `SphericalCubature` (for integrating over spheres and balls).

Please let me know if you find any mistakes. I will try to fix bugs when time is available.

Constructive comments for improvements are welcome; actually implementing any suggestions will be dependent on time constraints.

Version history:

- 1.0.1 original package
- 1.1 fix an incorrect test for dimension=1 in `SimplexVolume`; add functions `SimplexSurfaceArea`. Rename function `UnitSimplex` to `UnitSimplexV` to eliminate name conflict with function in package `mvmesh`.
- 1.2 miscellaneous small changes.
- 1.3 Eliminate internal function `integrate.vector.fn` and replace with a slightly different function `adaptIntegrateVectorFunc`. This new function is used in the new version of package `SphericalCubature`.

Author(s)

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References

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- N. Konerth, Exact integration on simplices, Undergraduate Research Paper, Math/Stat Department, American University (2014). Online at <http://aladinrc.wrlc.org/handle/1961/14863>

See Also

[adaptIntegrateSimplex](#), [integrateSimplexPolynomial](#)

adaptIntegrateSimplex *Integrate a general function over a simplex*

Description

Adaptive integration of a function $f(x)$ of n variables over an m -dimensional simplex S , $1 \leq m \leq n$. More generally, f can be a vector valued function and S can be a list of simplices.

Usage

```
adaptIntegrateSimplex(f, S, fDim = 1L, maxEvals = 10000L, absError = 0, tol = 1e-05,
  integRule = 3L, partitionInfo = FALSE, ...)
adaptIntegrateVectorFunc(intervals, fDim, f, maxEvals, absError, tol,
  partitionInfo=FALSE, ... )
original.coordinates( u, S )
```

Arguments

- | | |
|------|--|
| f | a function of n -variables (where n is determined by S) or a vector valued function (if $fDim > 1$). During the cubature process, f will be called with a single point x and it is assumed $f(x)$ returns a vector of length $fDim$. |
| S | a simplex or list of simplices that specify the region of integration. A single simplex S is given by an $n \times (m+1)$ matrix, where n is the dimension of the underlying space and m is the dimension of the simplex, $1 \leq m \leq n$. In this case, the columns $S[,1], \dots, S[,m+1]$ are the vertices of the m -dimensional simplex. If S is an $n \times (m+1) \times k$ array, then the region of integration is the union of the simplices $S[:,1], \dots, S[:,k]$, each of the above form. |
| fDim | integer dimension of the integrand function. |

<code>maxEvals</code>	integer maximum number of function evaluations allowed
<code>absError</code>	requested absolute error in the computation of the integral
<code>tol</code>	requested relative error in the computation of the integral
<code>integRule</code>	integer in the range 1:4 specifying degree of integration rule: a $(2*\text{integRule}+1)$ degree integration rule is used in function <code>adsimp</code> .
<code>partitionInfo</code>	if FALSE, then only the results of the computations are returned. If TRUE, then partition information is also returned for the final subdivision of the region. This will require more memory, but sometimes that information can be useful for other purposes.
<code>...</code>	optional arguments to integrand function <code>f(x,...)</code>
<code>intervals</code>	$(1 \times 2 \times k)$ array of intervals for univariate integration
<code>u</code>	point in m-dim. space

Details

If $m=n$, then an R translation of Alan Genz's function `adsimp(...)` is used to evaluate the n -dimensional integral. It works by adaptively splitting the region of integration into finer partitions, always splitting the simplex with the largest estimated error.

If $1 < m < n$, then the integral is evaluated by mapping the m -simplex in R^n to the canonical simplex in m -dimensional space, using function `adsimp` on that 'full' m -dimensional integral, and correcting with the Jacobian of the transformation.

If $m=1$, the function `adaptIntegrateVectorFunc` is used to evaluate the line integral. It uses the built-in R function `integrate` (from QUADPACK 1-dimensional adaptive quadrature) to evaluate the line integral. Since it does not provide access to the final subdivision, `partitionInfo=TRUE` in the univariate case returns the original partition information. So, if a fine partition is desired in the $m=1$ case, start with a fine partition. For consistency with `adaptIntegrateSimplex`, it is assumed that the integrand function `f` computes `fDim` values when called with a single `x` value. Since the `integrate` function does not handle vector integrands, the integration is done one coordinate at a time. This will be inefficient when `fDim > 1` and evaluation of `f` is complicated; consistent behavior of the integrand function was chosen over efficiency.

Value

A list containing:

<code>integral</code>	estimated value of the integral, it is a vector if <code>fDim > 1</code>
<code>estAbsError</code>	estimated absolute error
<code>functionEvaluations</code>	count of number of function evaluations
<code>returnCode</code>	integer status: <code>returnCode=0</code> is a successful return; non-zero error values are described by next variable
<code>message</code>	text message explaining <code>returnCode</code> ; "OK" for normal return
<code>subsimplices</code>	if <code>partitionInfo=TRUE</code> , this gives an array of subsimplices, see function <code>adsimp</code> for more details.

subsimplicesIntegral
 if partitionInfo=TRUE, this array gives estimated values of each component of the integral on each subsimplex, see function adsimp for more details.

subsimplicesAbsError
 if partitionInfo=TRUE, this array gives estimated values of the absolute error of each component of the integral on each subsimplex, see function adsimp for more details.

subsimplicesVolume
 if partitionInfo=TRUE, vector of m-dim. volumes of subsimplices; this is not d-dim. volume if $m < n$.

Note

No check is done on the simplices to see that they are disjoint.

When $m > 1$ and $fDim > 1$, adsimp uses the same grid for each coordinate of f .

When $m=1$ and $fDim > 1$, the components of the integral are evaluated independently, with an upper limit of maxEvals function evaluations for each component. This means that (a) a different grid may be used for each component, and (b) the return variable functionEvaluations is the sum of the number of function evaluations for each component; it may be up to $maxEvals * fDim$.

In keeping with Genz's original code, the vertices of the simplex described by S are column vectors, not row vectors.

References

See references to Genz and Cool (2003) in [SimplicialCubature-package](#).

Examples

```
n <- 4
S <- CanonicalSimplex( n )
f1 <- function( x ) { x[1]^3 }
adaptIntegrateSimplex( f1, S ) # correct answer 0.00119047619
str( adaptIntegrateSimplex( f1, S, partitionInfo=TRUE ) ) # same result, with more info returned

# test with vector valued integrand
f2 <- function( x ) { c(x[1]^3,x[3]^4) }
adaptIntegrateSimplex( f2, S, fDim=2 ) # correct answer 0.00119047619 0.0005952380952

# test with vector valued integrand and extra arguments
f3 <- function( x, extra.arg ) { extra.arg*c(x[1]^3,x[3]^4) } # multiple of f2 above
adaptIntegrateSimplex( f3, S, fDim=2, extra.arg=100 ) # correct answer 0.119047619 0.05952380952

# integrate over lower dimensional simplices
adaptIntegrateSimplex( f1, UnitSimplexV(4) ) # answer = 0.01666667

f4 <- function(x) { 1 }
# 2-dim integral, exact answer area of unit simplex = sqrt(3)/2 = 0.8660254...
adaptIntegrateSimplex( f4, UnitSimplexV(3) )

# line integral over diamond in 2-dim, exact answer=arclength=4*sqrt(2)=5.656854...
```

```
S4 <- array( c( 1,0, 0,1, 0,1, -1,0, -1,0, 0,-1, 0,-1, 1,0) , dim=c(2,2,4) )
adaptIntegrateSimplex( f4, S4 )
adaptIntegrateSimplex( f4, S4, partitionInfo=TRUE )
```

adsimp

Internal functions for adaptIntegrateSimplex.

Description

adsimp is a translation of Alan Genz's matlab program adsimp.m to adaptively integrate over a simplex. The other functions listed below are all called by adsimp. These functions are used internally; use at your own risk.

Usage

```
adsimp(ND, VRTS, NF, F, MXFS, EA, ER, KEY, partitionInfo = FALSE )
adsimp.return.message( rcode )
SMPCHC(ND, NF, MXFS, EA, ER, SBS, KEY)
SMPDFS(ND, NF, F, TOP, SBS, VRTS)
SMPRMS(N, KEY)
SMPRUL(ND, VRTS, VOL, NF, F, G, W, PTS)
SMPSAD(ND, NF, F, MXFS, EA, ER, KEY, RCLS, SBS, VRTS, partitionInfo )
SMPSMS(N, VERTEX, NF, F, G)
```

Arguments

ND, N	dimension of the space
VRTS, VERTEX	array specifying the simplices
NF	dimension of the function; F(x) has NF coordinates
F	a function of ND variables, value F(x) has NF coordinates
rcode	an integer return code from adsimp
MXFS	maximum number of function evaluations allowed
EA	requested absolute error
ER	requested relative error
KEY	integration rule
partitionInfo	TRUE or FALSE, controls whether or not the function returns information about the final partition. See the comments in function adaptIntegrateSimplex().
SBS	number of subsimplices
TOP	pointer to a subsimplex
VOL	volume of a simplex
G	generators for integration rule
W	weights for an integration rule
PTS	points in an integration rule
RCLS	number of terms in an integration rule

Value

Not meant to be used directly, these functions are generally called from function `adaptIntegrateSimplex(...)`.

See Also

[adaptIntegrateSimplex](#)

CanonicalSimplex

Internal functions for defining/working with simplices.

Description

These are utility functions that are useful when defining/working with simplices in n-dimensional space.

Usage

```
CanonicalSimplex(n)
UnitSimplexV(n)
SimplexVolume(S)
SimplexSurfaceArea(S3)
JacobianS2Canonical(S2)
```

Arguments

n	positive integer giving the dimension of the space
S	an n x (n+1) matrix specifying a single n-dimensional simplex; the columns S[,1],...,S[:,n+1] give the vertices of the simplex.
S2	an n x (m+1) matrix specifying a single m-dimensional simplex, with m <= n; the columns S2[,1],...,S2[:,m+1] give the vertices of the simplex.
S3	an n x n matrix specifying a single (n-1)-dimensional simplex inside n-dimensional space; the columns S3[,1],...,S3[:,n] give the vertices of the simplex.

Value

Let $e[j]$ be the j-th standard unit basis vector. `CanonicalSimplex(n)` gives the simplex with columns being vertices of the canonical simplex in n-dimensions: the n-dim. simplex with vertices $(0,0,\dots,0)$ and $e[1],\dots,e[n]$. A vector $(u[1],\dots,u[n])$ is in the canonical simplex if $0 \leq u[i] \leq 1$ for all i and $\text{sum}(u) \leq 1$. `UnitSimplexV(n)` gives the vertices (V-representation) of the unit simplex, namely $e[1],\dots,e[n]$. A vector $(u[1],\dots,u[n])$ is in the unit simplex if $0 \leq u[i] \leq 1$ for all i and $\text{sum}(u) = 1$. `SimplexVolume(S)` returns the n-dim. volume of S and `SimplexSurfaceArea(S3)` computes the (n-1)-dim. surface area of S3. `JacobianS2Canonical(S2)` returns the Jacobian of the transformation from an m-dim. simplex S2 to the m-dim. canonical simplex.

Examples

```

CanonicalSimplex(3)
UnitSimplexV(3)
SimplexVolume( CanonicalSimplex(3) )
SimplexSurfaceArea( UnitSimplexV(3) )
JacobianS2Canonical( UnitSimplexV(3) )

```

definePoly

Define, evaluate, or print a polynomial

Description

Utility functions to work with a multivariate polynomial.

Usage

```

definePoly(coef, k)
printPoly( p, num.digits )
evalPoly( x, p, useTerm=rep(TRUE, length(p$coef) ) )

```

Arguments

coef	a vector of coefficients, one for each term of p(x)
k	a matrix of (non-negative, integer) powers
p	a polynomial, defined by definePoly
num.digits	number of digits to print for the coefficients of the polynomial
x	a (n x m) matrix, with columns containing the vectors where the polynomial should be evaluated
useTerm	vector of boolean values: if useTerm[i]=TRUE, term i is included in the evaluation; if useTerm[i]=FALSE, term i is not included.

Details

These are utility functions for use with integrateSimplexPolynomial. definePoly is used to define a polynomial:

$$p(x) = \sum_{i=1}^{\text{length}(\text{coef})} \text{coef}_i x_1^{k[i,1]} x_2^{k[i,2]} \dots x_n^{k[i,n]}$$

printPoly prints a polynomial in human readable form.

evalPoly evaluates a polynomial at each of the vectors x[,1],x[,2],...,x[,m]. The optional argument useTerm is for internal use.

See example below.

Value

For `definePoly`, a list is returned. That list can be used by `integrateSimplexPolynomial`, `printPoly`, or `evalPoly`.

For `printPoly`, nothing is returned, but a human readable format is printed on the console.

For `evalPoly`, a vector of m values: $y[i] = p(x[,i])$.

Note

The internal definition of a polynomial may change in the future.

See Also

[integrateSimplexPolynomial](#)

Examples

```
p1 <- definePoly( c(3,5), matrix(c(3,0,0,0, 0,2,1,4), nrow=2, ncol=4, byrow=TRUE ) )
printPoly(p1)
evalPoly( c(1,3,1,2) , p1 ) # f(1,3,1,2) = 723
```

grnmol

Grundmann-Moller integration of a function over a simplex

Description

Computes an approximation to the integral of a function $f(x)$ over a simplex S . This is an R translation of the matlab function `grnmol.m` which was written by Alan Genz.

Usage

```
grnmol(f,V,s)
```

Arguments

<code>f</code>	a (real-valued) function f that can be evaluated at all points in V .
<code>V</code>	a single simplex, specified by an $(n \times (n+1))$ matrix. The columns $V[,1], \dots, V[,n+1]$ are the vertices of the simplex.
<code>s</code>	a positive integer specifying the order of the rule used

Details

The Grundmann-Moller algorithm approximates the integral of $f(x)$ over the simplex V . When $f(x)$ is a polynomial, and s is large enough, the integral is exact. This function is called by [integrateSimplexPolynomial](#).

Value

Q a vector of length $s+1$, with $Q[i]$ the i -th degree approximate value of the integral
 nv number of function evaluations used

References

See reference by Grundmann and Moller in [SimplicialCubature-package](#).

Examples

```
f <- function( x ) { x[1]^2*x[4]^5 }
grnmol( f, CanonicalSimplex(4), s=4 )
```

integrateSimplexPolynomial

Exact integration of a polynomial over a simplex

Description

Computes the exact integral of a polynomial $p(x)$ over an m -dimensional simplex S in n -dimensional space, $1 \leq m \leq n$. The methods are exact for polynomials, no approximation is used. The only inaccuracies possible are in the floating point evaluation of knots, coefficients, evaluation of the polynomial, sums, and products.

Usage

```
integrateSimplexPolynomial(p, S, method="GM")
```

Arguments

p a single polynomial, defined though function `definePoly`.
 S Either a single simplex, specified by an $n \times (m+1)$ matrix with the columns $S[,1], \dots, S[,n+1]$ giving the vertices of the simplex, or a $n \times (m+1) \times k$ array with $S[,1], \dots, S[,k]$ each a single simplex as described above.
 method either "GM" (for the Grundmann-Moller method) or "LA" (for the Lasserre-Avrenchenkov) method

Details

If `method="GM"`, the Grundmann-Moller method is used; it is exact for polynomials (because the function chooses a rule of high enough degree for the degree of the polynomial $p(x)$). This is faster, requiring fewer function evaluations. This method works for $n \geq 1$ and $1 \leq m \leq n$.

If `method="LA"`, the algorithm splits the polynomial into terms that are homogeneous of degree q , uses the method of Lasserre and Avrachonkov to exactly integrate those terms, and sums over all degrees. This method is slower, requiring more function evaluations. The degree of the polynomial has more effect on execution time than the number of terms or number of variables. This method only works with $n > 1$ and $m=n$.

Value

integral value of the integral
functionEvaluations
 number of function evaluations used

References

See references in [SimplicialCubature-package](#).

Examples

```
S <- CanonicalSimplex( 4 ) # 4-dim. simplex
p1 <- definePoly( 1.0, matrix( c(2,0,0,5), nrow=1 ) )
printPoly(p1)
# same as example for function grnmol( ), but explicitly using the fact that the integrand
# function is a polynomial, and automatic selection of the order of the integration rule
integrateSimplexPolynomial( p1, S, method="GM" )
integrateSimplexPolynomial( p1, S, method="LA" )

p2 <- definePoly( c(5,-6), matrix( c(3,1,0,0, 0,0,0,7), nrow=2, byrow=TRUE) )
printPoly( p2 )
integrateSimplexPolynomial( p2, S, method="GM" ) # correct answer -1.352814e-05
integrateSimplexPolynomial( p2, S, method="LA" ) # correct answer -1.352814e-05

# integrate random polynomials and random simplices in different dimensions
for (n in 3:5) {
  S <- matrix( rnorm(n*(n+1)), nrow=n, ncol=n+1 )
  p.rand <- definePoly( rnorm(1), matrix( c(4, rep(0,n-1)), nrow=1 ) )
  #printPoly(p.rand)
  tmp1 <- integrateSimplexPolynomial( p.rand, S, method="GM" )
  tmp2 <- integrateSimplexPolynomial( p.rand, S, method="LA" )
  cat("n=",n," GM integral=",tmp1$integral," functionEvaluations=",tmp1$functionEvaluations,
      " LA integral=", tmp2$integral, " functionEvaluations=",tmp2$functionEvaluations,"\n")
}
```

LasserreAvrachenkov *Internal functions for integrateSimplexPolynomial.*

Description

LasserreAvrachenkov implements the exact integration formula for a homogeneous polynomial p of degree q . The other functions are helper functions for that.

Usage

```
LasserreAvrachenkov(q, p, useTerm, S)  
nextIndexLA(current.n, b)  
nextIntBaseB(current.n, b)
```

Arguments

q	degree of the polynomial p
p	polynomial obtained by calling definePoly
useTerm	vector of booleans, telling which terms are homogeneous of degree q
S	an n x (n+1) matrix specifying a single simplex; the columns S[:,1],...,S[:,n+1] give the vertices of the simplex.
current.n	vector of integers giving the base b representation of a (non-negative) integer
b	base used for the base b representation of an integer

Value

Not meant to be called externally.

References

See Lasserre and Avrachenkov, Baldoni, et al., and Konerth references in [SimplicialCubature-package](#).

See Also

[integrateSimplexPolynomial](#)

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