Package 'fastGHQuad'

September 30, 2018

Type Package

Title Fast 'Rcpp' Implementation of Gauss-Hermite Quadrature

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Description Fast, numerically-stable Gauss-Hermite quadrature rules and utility functions for adaptive GH quadrature. See Liu, Q. and Pierce, D. A. (1994) <doi:10.2307/2337136> for a reference on these methods.

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LazyLoad yes

URL https://github.com/awblocker/fastGHQuad

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LinkingTo Rcpp

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NeedsCompilation yes

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R topics documented:

fastGHQuad-package *A package for fast, numerically-stable computation of Gauss-Hermite quadrature rules*

Description

This package provides functions to compute Gauss-Hermite quadrature rules very quickly with a higher degree of numerical stability (tested up to 2000 nodes).

Details

It also provides function for adaptive Gauss-Hermite quadrature, extending Laplace approximations (as in Liu & Pierce 1994).

Package:	fastGHQuad
Type:	Package
License:	MIT
LazyLoad:	yes

Author(s)

Alexander W Blocker

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References

Golub, G. H. and Welsch, J. H. (1969). Calculation of Gauss Quadrature Rules. Mathematics of Computation 23 (106): 221-230.

Liu, Q. and Pierce, D. A. (1994). A Note on Gauss-Hermite Quadrature. Biometrika, 81(3) 624-629.

See Also

gaussHermiteData, aghQuad, ghQuad

Examples

```
# Get quadrature rule
rule <- gaussHermiteData(1000)

# Find a normalizing constant
g <- function(x) 1/(1+x^2/10)^(11/2) # t distribution with 10 df
aghQuad(g, 0, 1.1, rule)
# actual is
1/dt(0,10)
```

```
# Find an expectation
g <- function(x) x^2*dt(x,10) # t distribution with 10 df
aghQuad(g, 0, 1.1, rule)
# actual is 1.25
```

---

aghQuad *Adaptive Gauss-Hermite quadrature using Laplace approximation*

Description

Convenience function for integration of a scalar function g based upon its Laplace approximation.

Usage

```
aghQuad(g, muHat, sigmaHat, rule, ...)
```

Arguments

g	Function to integrate with respect to first (scalar) argument
muHat	Mode for Laplace approximation
sigmaHat	Scale for Laplace approximation (`sqrt(-1/H)`, where H is the second derivative of log(g) at muHat)
rule	Gauss-Hermite quadrature rule to use, as produced by `gaussHermiteData`
...	Additional arguments for g

Details

This function approximates

$$\int_{-\infty}^{\infty} g(x)\, dx$$

using the method of Liu & Pierce (1994). This technique uses a Gaussian approximation of g (or the distribution component of g, if an expectation is desired) to "focus" quadrature around the high-density region of the distribution. Formally, it evaluates:

$$\sqrt{2}\hat{\sigma} \sum_i w_i \exp(x_i^2) g(\hat{\mu} + \sqrt{2}$$

$$\hat{\sigma} x_i)$$

where x and w come from the given rule.

This method can, in many cases (where the Gaussian approximation is reasonably good), achieve better results with 10-100 quadrature points than with 1e6 or more draws for Monte Carlo integration. It is particularly useful for obtaining marginal likelihoods (or posteriors) in hierarchical and multilevel models — where conditional independence allows for unidimensional integration, adaptive Gauss-Hermite quadrature is often extremely effective.

Value

Numeric (scalar) with approximation integral of g from -Inf to Inf.

Author(s)

Alexander W Blocker <ablocker@gmail.com>

References

Liu, Q. and Pierce, D. A. (1994). A Note on Gauss-Hermite Quadrature. Biometrika, 81(3) 624-629.

See Also

gaussHermiteData, ghQuad

Examples

```
# Get quadrature rules
rule10  <- gaussHermiteData(10)
rule100 <- gaussHermiteData(100)

# Estimating normalizing constants
g <- function(x) 1/(1+x^2/10)^(11/2) # t distribution with 10 df
aghQuad(g, 0, 1.1,  rule10)
aghQuad(g, 0, 1.1,  rule100)
# actual is
1/dt(0,10)

# Can work well even when the approximation is not exact
g <- function(x) exp(-abs(x)) # Laplace distribution
aghQuad(g, 0, 2,  rule10)
aghQuad(g, 0, 2,  rule100)
# actual is 2

# Estimating expectations
# Variances for the previous two distributions
g <- function(x) x^2*dt(x,10) # t distribution with 10 df
aghQuad(g, 0, 1.1,  rule10)
aghQuad(g, 0, 1.1,  rule100)
# actual is 1.25

# Can work well even when the approximation is not exact
g <- function(x) x^2*exp(-abs(x))/2 # Laplace distribution
aghQuad(g, 0, 2,  rule10)
aghQuad(g, 0, 2,  rule100)
# actual is 2
```

evalHermitePoly — *Evaluate Hermite polynomial at given location*

Description

Evaluate Hermite polynomial of given degree at given location. This function is provided for demonstration/teaching purposes; this method is not used by gaussHermiteData. It is numerically unstable for high-degree polynomials.

Usage

```
evalHermitePoly(x, n)
```

Arguments

`x`	Vector of location(s) at which polynomial will be evaluated
`n`	Degree of Hermite polynomial to compute

Value

Vector of length(x) values of Hermite polynomial

Author(s)

Alexander W Blocker <ablocker@gmail.com>

See Also

gaussHermiteData, aghQuad, ghQuad

findPolyRoots — *Find real parts of roots of polynomial*

Description

Finds real parts of polynomial's roots via eigendecomposition of companion matrix. This method is not used by gaussHermiteData. Only the real parts of each root are retained; this can be useful if the polynomial is known a priori to have all roots real.

Usage

```
findPolyRoots(c)
```

Arguments

`c`	Coefficients of polynomial

Value

Numeric vector containing the real parts of the roots of the polynomial defined by c

Author(s)

Alexander W Blocker <ablocker@gmail.com>

See Also

gaussHermiteData, aghQuad, ghQuad

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gaussHermiteData *Compute Gauss-Hermite quadrature rule*

Description

Computes Gauss-Hermite quadrature rule of requested order using Golub-Welsch algorithm. Returns result in list consisting of two entries: x, for nodes, and w, for quadrature weights. This is very fast and numerically stable, using the Golub-Welsch algorithm with specialized eigendecomposition (symmetric tridiagonal) LAPACK routines. It can handle quadrature of order 1000+.

Usage

```
gaussHermiteData(n)
```

Arguments

n	Order of Gauss-Hermite rule to compute (number of nodes)

Details

This function computes the Gauss-Hermite rule of order n using the Golub-Welsch algorithm. All of the actual computation is performed in C/C++ and FORTRAN (via LAPACK). It is numerically-stable and extremely memory-efficient for rules of order 1000+.

Value

A list containing:

x	the n node positions for the requested rule
w	the w quadrature weights for the requested rule

Author(s)

Alexander W Blocker <ablocker@gmail.com>

References

Golub, G. H. and Welsch, J. H. (1969). Calculation of Gauss Quadrature Rules. Mathematics of Computation 23 (106): 221-230

Liu, Q. and Pierce, D. A. (1994). A Note on Gauss-Hermite Quadrature. Biometrika, 81(3) 624-629.

See Also

aghQuad, ghQuad

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ghQuad — *Convenience function for Gauss-Hermite quadrature*

Description

Convenience function for evaluation of Gauss-Hermite quadrature

Usage

```
ghQuad(f, rule, ...)
```

Arguments

`f`	Function to integrate with respect to first (scalar) argument; this does not include the weight function `exp(-x^2)`
`rule`	Gauss-Hermite quadrature rule to use, as produced by `gaussHermiteData`
`...`	Additional arguments for f

Details

This function performs classical unidimensional Gauss-Hermite quadrature with the function f using the rule provided; that is, it approximates

$$\int_{-\infty}^{\infty} f(x) \exp(-x^2) \, dx$$

by evaluating

$$\sum_i w_i f(x_i)$$

Value

Numeric (scalar) with approximation integral of f(x)*exp(-x^2) from -Inf to Inf.

Author(s)

Alexander W Blocker <ablocker@gmail.com>

References

Golub, G. H. and Welsch, J. H. (1969). Calculation of Gauss Quadrature Rules. Mathematics of Computation 23 (106): 221-230.

Liu, Q. and Pierce, D. A. (1994). A Note on Gauss-Hermite Quadrature. Biometrika, 81(3) 624-629.

See Also

gaussHermiteData, ghQuad

Examples

```
# Get quadrature rules
rule10  <- gaussHermiteData(10)
rule100 <- gaussHermiteData(100)

# Check that rule is implemented correctly
f <- function(x) rep(1,length(x))
if (!isTRUE(all.equal(sqrt(pi), ghQuad(f, rule10), ghQuad(f, rule100)))) {
  print(ghQuad(f, rule10))
  print(ghQuad(f, rule100))
}
# These should be 1.772454

f <- function(x) x
if (!isTRUE(all.equal(0.0, ghQuad(f, rule10), ghQuad(f, rule100)))) {
  print(ghQuad(f, rule10))
  print(ghQuad(f, rule100))
}
# These should be zero
```

---

hermitePolyCoef *Get coefficient of Hermite polynomial*

Description

Calculate coefficients of Hermite polynomial using recursion relation. This function is provided for demonstration/teaching purposes; this method is not used by gaussHermiteData. It is numerically unstable for high-degree polynomials.

Usage

```
hermitePolyCoef(n)
```

Arguments

`n` Degree of Hermite polynomial to compute

Value

Vector of (n+1) coefficients from requested polynomial

Author(s)

Alexander W Blocker <ablocker@gmail.com>

See Also

gaussHermiteData, aghQuad, ghQuad

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