Package 'aghq'

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Description Adaptive Gauss Hermite Quadrature for Bayesian inference. The AGHQ method for normalizing posterior distributions and making Bayesian inferences based on them. Functions are provided for doing quadrature and marginal Laplace approximations, and summary methods are provided for making inferences based on the results. See Stringer (2021). ``Implementing Adaptive Quadrature for Bayesian Inference: the aghq Package" <arxiv:2101.04468>.</arxiv:2101.04468>
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Adaptive Gauss-Hermite Quadrature

Description

Normalize the log-posterior distribution using Adaptive Gauss-Hermite Quadrature. This function takes in a function and its gradient and Hessian, and returns a list of information about the normalized posterior, with methods for summarizing and plotting.

Usage

```
aghq(
   ff,
   k,
   startingvalue,
   optresults = NULL,
   basegrid = NULL,
   control = default_control(),
   ...
)
```

Arguments

ff

A list with three elements:

- fn: function taking argument theta and returning a numeric value representing the log-posterior at theta
- gr: function taking argument theta and returning a numeric vector representing the gradient of the log-posterior at theta
- he: function taking argument theta and returning a numeric matrix representing the hessian of the log-posterior at theta

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> The user may wish to use numDeriv::grad and/or numDeriv::hessian to obtain these. Alternatively, the user may consider the TMB package. This list is deliberately formatted to match the output of TMB:: MakeADFun.

Integer, the number of quadrature points to use. I suggest at least 3. k = 1corresponds to a Laplace approximation.

Value to start the optimization. ff\$fn(startingvalue), ff\$gr(startingvalue), and ff\$he(startingvalue) must all return appropriate values without error.

Optional. A list of the results of the optimization of the log posterior, formatted according to the output of aghq::optimize_theta. The aghq::aghq function handles the optimization for you; passing this list overrides this, and is useful for when you know your optimization is too difficult to be handled by generalpurpose software. See the software paper for several examples of this. If you're unsure whether this option is needed for your problem then it probably is not.

Optional. Provide an object of class NIGrid from the mvQuad package, representing the base quadrature rule that will be adapted. This is only for users who want more complete control over the quadrature, and is not necessary if you are fine with the default option which basically corresponds to mvQuad::createNIGrid(length(theta)

Note: the mvQuad functions used within aghq operate on grids in memory, so your basegrid object will be changed after you run aghq.

control A list with elements

• method: optimization method to use:

- 'sparse_trust' (default): trustOptim::trust.optim with method = 'sparse'

- 'SR1' (default): trustOptim::trust.optim with method = 'SR1'

- 'trust': trust::trust

- 'BFGS': optim(..., method = "BFGS")

Default is 'sparse_trust'.

• optcontrol: optional: a list of control parameters to pass to the internal optimizer you chose. The aghq package uses sensible defaults.

Additional arguments to be passed to ff\$fn, ff\$gr, and ff\$he.

Details

When k = 1 the AGHQ method is a Laplace approximation, and you should use the aghq::laplace_approximation function, since some of the methods for aghq objects won't work with only one quadrature point. Objects of class laplace have different methods suited to this case. See ?aghq::laplace_approximation.

Value

An object of class aghq which is a list containing elements:

- normalized_posterior: The output of the normalize_logpost function, which itself is a list with elements:
 - nodesandweights: a dataframe containing the nodes and weights for the adaptive quadrature rule, with the un-normalized and normalized log posterior evaluated at the nodes.
 - thegrid: a NIGrid object from the mvQuad package, see ?mvQuad::createNIGrid.
 - lognormconst: the actual result of the quadrature: the log of the normalizing constant of the posterior.
- marginals: a list of the same length as startingvalue of which element j is the result of calling aghq::marginal_posterior with that j. This is a tbl_df/tbl/data.frame containing the normalized log marginal posterior for theta_j evaluated at the original quadrature points. Has columns "thetaj", "logpost_normalized", "weights", where j is the j you specified.

startingvalue

optresults

k

basegrid

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• optresults: information and results from the optimization of the log posterior, the result of calling aghq::optimize_theta. This a list with elements:

- ff: the function list that was provided
- mode: the mode of the log posterior
- hessian: the hessian of the log posterior at the mode
- convergence: specific to the optimizer used, a message indicating whether it converged
- control: the control parameters passed

See Also

```
Other quadrature: get_log_normconst(), laplace_approximation(), marginal_laplace_tmb(), marginal_laplace(), normalize_logpost(), optimize_theta(), plot.aghq(), print.aghqsummary(), print.aghq(), print.laplacesummary(), print.laplace(), print.marginallaplacesummary(), summary.aghq(), summary.laplace(), summary.marginallaplace()
```

Examples

```
logfteta2d <- function(eta,y) {</pre>
  # eta is now (eta1,eta2)
  # y is now (y1,y2)
  n <- length(y)</pre>
  n1 <- ceiling(n/2)
  n2 \leftarrow floor(n/2)
  y1 <- y[1:n1]
  y2 \leftarrow y[(n1+1):(n1+n2)]
  eta1 <- eta[1]
  eta2 <- eta[2]
  sum(y1) * eta1 - (length(y1) + 1) * exp(eta1) - sum(lgamma(y1+1)) + eta1 +
    sum(y2) * eta2 - (length(y2) + 1) * exp(eta2) - sum(lgamma(y2+1)) + eta2
set.seed(84343124)
n1 <- 5
n2 <- 5
n < - n1+n2
y1 <- rpois(n1,5)
y2 \leftarrow rpois(n2,5)
objfunc2d <- function(x) logfteta2d(x,c(y1,y2))
funlist2d <- list(</pre>
  fn = objfunc2d,
  gr = function(x) numDeriv::grad(objfunc2d,x),
  he = function(x) numDeriv::hessian(objfunc2d,x)
thequadrature <- aghq(funlist2d,3,c(0,0))</pre>
```

compute_moment

Compute moments

Description

Compute the moment of any function ff using AGHQ.

compute_moment 5

Usage

```
compute_moment(obj, ...)
## Default S3 method:
compute_moment(obj, ff = function(x) 1, ...)
## S3 method for class 'aghq'
compute_moment(obj, ff = function(x) 1, ...)
```

Arguments

obj	Object of class aghq output by aghq::aghq(), or its normalized_posterior element. See ?aghq.
	Used to pass additional argument ff.
ff	Any R function which takes in a numeric vector and returns a numeric vector.

Value

A numeric vector containing the moment(s) of ff with respect to the joint distribution being approximated using AGHQ.

See Also

```
Other summaries: compute_pdf_and_cdf(), compute_quantiles(), interpolate_marginal_posterior(), marginal_posterior()
```

```
logfteta2d <- function(eta,y) {</pre>
  # eta is now (eta1,eta2)
  # y is now (y1,y2)
  n <- length(y)</pre>
  n1 <- ceiling(n/2)</pre>
  n2 \leftarrow floor(n/2)
  y1 <- y[1:n1]
  y2 \leftarrow y[(n1+1):(n1+n2)]
  eta1 <- eta[1]
  eta2 <- eta[2]
  sum(y1) * eta1 - (length(y1) + 1) * exp(eta1) - sum(lgamma(y1+1)) + eta1 +
    sum(y2) * eta2 - (length(y2) + 1) * exp(eta2) - sum(lgamma(y2+1)) + eta2
set.seed(84343124)
n1 <- 5
n2 <- 5
n < - n1+n2
y1 <- rpois(n1,5)
y2 \leftarrow rpois(n2,5)
objfunc2d <- function(x) logfteta2d(x,c(y1,y2))
funlist2d <- list(</pre>
  fn = objfunc2d,
  gr = function(x) numDeriv::grad(objfunc2d,x),
  he = function(x) numDeriv::hessian(objfunc2d,x)
opt_sparsetrust_2d <- optimize_theta(funlist2d,c(1.5,1.5))</pre>
```

```
norm_sparse_2d_7 <- normalize_logpost(opt_sparsetrust_2d,7,1)

# ff = function(x) 1 should return 1,
# the normalizing constant of the (already normalized) posterior:
compute_moment(norm_sparse_2d_7)
# Compute the mean of theta1 and theta2
compute_moment(norm_sparse_2d_7,ff = function(x) x)
# Compute the mean of lambda1 = exp(theta1) and lambda2 = exp(theta2)
lambdameans <- compute_moment(norm_sparse_2d_7,ff = function(x) exp(x))
lambdameans
# Compare them to the truth:
(sum(y1) + 1)/(length(y1) + 1)
(sum(y2) + 1)/(length(y2) + 1)
# Compute the standard deviation of lambda1
lambda1sd <- sqrt(compute_moment(norm_sparse_2d_7,ff = function(x) (exp(x) - lambdameans[1])^2))[1]
# ...and so on.</pre>
```

Density and Cumulative Distribution Function

Description

Compute the density and cumulative distribution function of the approximate posterior. The density is approximated on a find grid using a polynomial interpolant. The CDF can't be computed exactly (if it could, you wouldn't be using quadrature!), so a fine grid is laid down and the CDF is approximated at each grid point using a simpler integration rule and a polynomial interpolant. This method tends to work well, but won't always.

Usage

```
compute_pdf_and_cdf(obj, ...)
## Default S3 method:
compute_pdf_and_cdf(
  obj,
  transformation = NULL,
  finegrid = NULL,
  interpolation = "auto",
  ...
)
## S3 method for class 'list'
compute_pdf_and_cdf(obj, ...)
## S3 method for class 'aghq'
compute_pdf_and_cdf(obj, ...)
```

Arguments

obj

Either the output of aghq::aghq(), its list of marginal distributions (element marginals), or an individual data.frame containing one of these marginal distributions as output by aghq::marginal_posterior().

... Used to pass additional arguments.

transformation Optional. A list containing two functions, fromtheta and totheta, which ac-

cept and return numeric vectors, defining a parameter transformation for which you would also like the pdf calculated for. See examples. May also have an element jacobian, a function which takes a numeric vector and computes the jacobian of the transformation; if not provided, this is done using numDeriv::jacobian.

finegrid Optional, a grid of values on which to compute the CDF. The default makes

use of the values in margpost but if the results are unsuitable, you may wish to

modify this manually.

interpolation Which method to use for interpolating the marginal posterior, 'polynomial'

(default) or 'spline'? If k>3 then the polynomial may be unstable and you should use the spline, but the spline doesn't work *unless* k>3 so it's not the

default. See interpolate_marginal_posterior().

Value

A tbl_df/tbl/data.frame with columns theta, pdf and cdf corresponding to the value of the parameter and its estimated PDF and CDF at that value.

See Also

Other summaries: compute_moment(), compute_quantiles(), interpolate_marginal_posterior(), marginal_posterior()

```
logfteta2d <- function(eta,y) {</pre>
  # eta is now (eta1,eta2)
  # y is now (y1,y2)
  n <- length(y)</pre>
  n1 <- ceiling(n/2)</pre>
  n2 \leftarrow floor(n/2)
  y1 <- y[1:n1]
  y2 \leftarrow y[(n1+1):(n1+n2)]
  eta1 <- eta[1]
  eta2 <- eta[2]
  sum(y1) * eta1 - (length(y1) + 1) * exp(eta1) - sum(lgamma(y1+1)) + eta1 +
    sum(y2) * eta2 - (length(y2) + 1) * exp(eta2) - sum(lgamma(y2+1)) + eta2
}
set.seed(84343124)
n1 <- 5
n2 <- 5
n <- n1+n2
y1 <- rpois(n1,5)
y2 <- rpois(n2,5)
objfunc2d <- function(x) logfteta2d(x,c(y1,y2))
funlist2d <- list(</pre>
  fn = objfunc2d,
  gr = function(x) numDeriv::grad(objfunc2d,x),
  he = function(x) numDeriv::hessian(objfunc2d,x)
opt_sparsetrust_2d <- optimize_theta(funlist2d,c(1.5,1.5))</pre>
margpost <- marginal_posterior(opt_sparsetrust_2d,3,1) # margpost for theta1</pre>
thepdfandcdf <- compute_pdf_and_cdf(margpost)</pre>
with(thepdfandcdf,{
```

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```
plot(pdf~theta,type='l')
plot(cdf~theta,type='l')
})
```

compute_quantiles

Quantiles

Description

Compute marginal quantiles using AGHQ. This function works by first approximating the CDF using aghq::compute_pdf_and_cdf and then inverting the approximation numerically.

Usage

```
compute_quantiles(obj, ...)

## Default S3 method:
compute_quantiles(
  obj,
  q = c(0.025, 0.975),
  transformation = NULL,
  interpolation = "polynomial",
  ...
)

## S3 method for class 'list'
compute_quantiles(obj, q = c(0.025, 0.975), transformation = NULL, ...)

## S3 method for class 'aghq'
compute_quantiles(obj, q = c(0.025, 0.975), transformation = NULL, ...)
```

Arguments

obj Either the output of aghq::aghq(), its list of marginal distributions (element marginals), or an individual data.frame containing one of these marginal dis-

tributions as output by aghq::marginal_posterior().

... Used to pass additional arguments.

q Numeric vector of values in (0,1). The quantiles to compute.

transformation Optional. A list containing function fromtheta() which accepts and returns

numeric vectors, defining a parameter transformation for which you would like the quantiles of. See ?compute_pdf_and_cdf. This transformation must be monotone and the function checks whether it's increasing or decreasing and

returns the transformed quantiles, ordered appropriately.

interpolation Which method to use for interpolating the marginal posterior, 'polynomial'

(default) or 'spline'? If k > 3 then the polynomial may be unstable and you should use the spline, but the spline doesn't work *unless* k > 3 so it's not the

default. See interpolate_marginal_posterior().

default_control 9

Value

A named numeric vector containing the quantiles you asked for, for the variable whose marginal posterior you provided.

See Also

```
Other summaries: compute_moment(), compute_pdf_and_cdf(), interpolate_marginal_posterior(), marginal_posterior()
```

```
logfteta2d <- function(eta,y) {</pre>
  # eta is now (eta1,eta2)
  # y is now (y1,y2)
  n <- length(y)</pre>
  n1 <- ceiling(n/2)</pre>
  n2 \leftarrow floor(n/2)
  y1 <- y[1:n1]
  y2 \leftarrow y[(n1+1):(n1+n2)]
  eta1 <- eta[1]
  eta2 <- eta[2]
  sum(y1) * eta1 - (length(y1) + 1) * exp(eta1) - sum(lgamma(y1+1)) + eta1 +
    sum(y2) * eta2 - (length(y2) + 1) * exp(eta2) - sum(lgamma(y2+1)) + eta2
set.seed(84343124)
n1 <- 5
n2 <- 5
n <- n1+n2
y1 <- rpois(n1,5)
y2 \leftarrow rpois(n2,5)
objfunc2d <- function(x) logfteta2d(x,c(y1,y2))
funlist2d <- list(</pre>
  fn = objfunc2d,
  gr = function(x) numDeriv::grad(objfunc2d,x),
  he = function(x) numDeriv::hessian(objfunc2d,x)
opt_sparsetrust_2d <- optimize_theta(funlist2d,c(1.5,1.5))</pre>
margpost <- marginal_posterior(opt_sparsetrust_2d,3,1) # margpost for theta1</pre>
etaquant <- compute_quantiles(margpost)</pre>
etaquant
\# lambda = exp(eta)
exp(etaquant)
# Compare to truth
qgamma(.025,1+sum(y1),1+n1)
qgamma(.975, 1+sum(y1), 1+n1)
```

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Description

Run default_control() to print the list of valid control parameters and their defaults, and run with named arguments to change the defaults.

Usage

```
default_control(...)
```

Arguments

You can provide a named value for any control parameter and its value will be set accordingly. See ?aghq and examples here.

Details

Valid options are:

• method: optimization method to use:

```
- 'BFGS' (default): optim(...,method = "BFGS")
- 'sparse_trust': trustOptim::trust.optim
- 'SR1': trustOptim::trust.optim with method = 'SR1'
- 'sparse': trust::trust
```

Default is 'sparse_trust'.

- negate: default FALSE. Multiply the functions in ff by -1? The reason for having this option is for full compatibility with TMB: while of course TMB allows you to code up your log-posterior any way you like, all of its excellent features including its automatic Laplace approximation and MCMC sampling with tmbstan assume you have coded your template to return the **negated** log-posterior. However, by default, aghq assumes you have provided the log-posterior without negation. Set negate = TRUE if you have provided a template which computes the negated log-posterior and its derivatives.
- ndConstruction: construct a multivariate quadrature rule using a "product" rule or a "sparse" grid? Default "product". See ?mvQuad::createNIGrid().
- interpolation: how to interpolate the marginal posteriors. The 'auto' option (default) chooses for you and should always work well. The 'polynomial' option uses polynom::poly.calc() to construct a global polynomial interpolant and has been observed to be unstable as the number of quadrature points gets larger, which is obviously a bad thing. Try 'spline' instead, which uses a cubic B-Spline interpolant from splines::interpSpline().
- numbersian: logical, default FALSE. Replace the ff\$he with a numerically-differentiated version, by calling numDeriv::jacobian on ff\$gr. Used mainly for TMB with the automatic Laplace approximation, which does not have an automatic Hessian.
- onlynormconst: logical, default FALSE. Skip everything after the calculation of the log integral, and just return the numeric value of the log integral. Saves computation time, and most useful in cases where aghq is being used as a step in a more complicated procedure.

Value

A list of argument values.

Examples

```
default_control()
default_control(method = "trust")
default_control(negate = TRUE)
```

```
default_control_marglaplace
```

Default control arguments for aghq::marginal_laplace().

Description

Run default_control_marglaplace() to print the list of valid control parameters and their defaults, and run with named arguments to change the defaults.

Usage

```
default_control_marglaplace(...)
```

Arguments

You can provide a named value for any control parameter and its value will be set accordingly. See ?marginal_laplace and examples here.

Details

Valid options are:

- method: optimization method to use for the theta optimization:
 - 'BFGS' (default): optim(...,method = "BFGS")
 'sparse_trust': trustOptim::trust.optim
 'SR1': trustOptim::trust.optim with method = 'SR1'
 'sparse': trust::trust
- inner_method: optimization method to use for the W optimization; same options as for method. Default inner_method is 'sparse_trust' and default method is 'BFGS'.
- negate: default FALSE. Multiply the functions in ff by -1? The reason for having this option is for full compatibility with TMB: while of course TMB allows you to code up your log-posterior any way you like, all of its excellent features including its automatic Laplace approximation and MCMC sampling with tmbstan assume you have coded your template to return the **negated** log-posterior. However, by default, aghq assumes you have provided the log-posterior **without negation**. Set negate = TRUE if you have provided a template which computes the **negated** log-posterior and its derivatives. **Note** that I don't expect there to be any reason to need this argument for marginal_laplace; if you are doing a marginal Laplace approximation using the automatic Laplace approximation provided by TMB, you should check out aghq::marginal_laplace_tmb().
- interpolation: how to interpolate the marginal posteriors. The 'auto' option (default) chooses for you and should always work well. The 'polynomial' option uses polynom::poly.calc() to construct a global polynomial interpolant and has been observed to be unstable as the number of quadrature points gets larger, which is obviously a bad thing. Try 'spline' instead, which uses a cubic B-Spline interpolant from splines::interpSpline().

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• numbersian: logical, default FALSE. Replace the ff\$he with a numerically-differentiated version, by calling numDeriv::jacobian on ff\$gr. Used mainly for TMB with the automatic Laplace approximation, which does not have an automatic Hessian.

• onlynormconst: logical, default FALSE. Skip everything after the calculation of the log integral, and just return the numeric value of the log integral. Saves computation time, and most useful in cases where aghq is being used as a step in a more complicated procedure.

Value

A list of argument values.

Examples

```
default_control_marglaplace()
default_control_marglaplace(method = "trust")
default_control_marglaplace(method = "trust",inner_method = "trust")
default_control_marglaplace(negate = TRUE)
```

default_control_tmb

Default control arguments for aghq::marginal_laplace_tmb().

Description

Run default_control_marglaplace() to print the list of valid control parameters and their defaults, and run with named arguments to change the defaults.

Usage

```
default_control_tmb(...)
```

Arguments

You can provide a named value for any control parameter and its value will be set accordingly. See ?marginal_laplace and examples here.

Details

Valid options are:

• method: optimization method to use for the theta optimization:

```
- 'BFGS' (default): optim(...,method = "BFGS")
- 'sparse_trust': trustOptim::trust.optim
- 'SR1': trustOptim::trust.optim with method = 'SR1'
- 'sparse': trust::trust
```

• negate: default TRUE. Assumes that your TMB function template computes the **negated** log-posterior, which it must if you're using TMB's automatic Laplace approximation, which you must be if you're using this function!.

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• interpolation: how to interpolate the marginal posteriors. The 'auto' option (default) chooses for you and should always work well. The 'polynomial' option uses polynom::poly.calc() to construct a global polynomial interpolant and has been observed to be unstable as the number of quadrature points gets larger, which is obviously a bad thing. Try 'spline' instead, which uses a cubic B-Spline interpolant from splines::interpSpline().

- numbersian: logical, default TRUE. Replace the ff\$he with a numerically-differentiated version, by calling numDeriv::jacobian on ff\$gr. Used mainly for TMB with the automatic Laplace approximation, which does not have an automatic Hessian.
- onlynormconst: logical, default FALSE. Skip everything after the calculation of the log integral, and just return the numeric value of the log integral. Saves computation time, and most useful in cases where aghq is being used as a step in a more complicated procedure.

Value

A list of argument values.

Examples

```
default_control_marglaplace()
default_control_marglaplace(method = "trust")
default_control_marglaplace(method = "trust",inner_method = "trust")
default_control_marglaplace(negate = TRUE)
```

gcdata

Globular Clusters data for Milky Way mass estimation

Description

Measurements on star clusters from Eadie and Harris (2016), for use within the Milky Way mass estimation example. Data are documented extensively by that source.

Usage

gcdata

Format

An object of class tbl_df (inherits from tbl, data.frame) with 70 rows and 25 columns.

Source

Eadie GM, Harris WE (2016). "Bayesian mass estimates of the Milky Way: the dark and light sides of parameter assumptions." The Astrophysical Journal, 829(108).

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gcdatalist

Transformed Globular Clusters data

Description

GC data prepared for input into the TMB template, for purposes of example. There are a lot of example-specific data preprocessing steps that are not related to the AGHQ method, so for brevity these are done beforehand.

Usage

gcdatalist

Format

An object of class list of length 6.

Source

Eadie GM, Harris WE (2016). "Bayesian mass estimates of the Milky Way: the dark and light sides of parameter assumptions." The Astrophysical Journal, 829(108).

get_log_normconst

Obtain the log-normalizing constant from a fitted quadrature object

Description

Quick helper S3 method to retrieve the log normalizing constant from an object created using the aghq package. Methods for a list (returned by aghq::normalize_posterior) and for objects of class aghq, laplace, and marginallaplace.

Usage

```
get_log_normconst(obj, ...)
## Default S3 method:
get_log_normconst(obj, ...)
## S3 method for class 'numeric'
get_log_normconst(obj, ...)
## S3 method for class 'aghq'
get_log_normconst(obj, ...)
## S3 method for class 'laplace'
get_log_normconst(obj, ...)
## S3 method for class 'marginallaplace'
get_log_normconst(obj, ...)
```

Arguments

```
obj A list returned by aghq::normalize_posterior or an object of class aghq, laplace, or marginallaplace.

Not used
```

Value

A number representing the natural logarithm of the approximated normalizing constant.

See Also

```
Other quadrature: aghq(), laplace_approximation(), marginal_laplace_tmb(), marginal_laplace(), normalize_logpost(), optimize_theta(), plot.aghq(), print.aghqsummary(), print.aghq(), print.laplacesummary(), print.laplace(), print.marginallaplacesummary(), summary.aghq(), summary.laplace(), summary.marginallaplace()
```

```
interpolate_marginal_posterior
```

Interpolate the Marginal Posterior

Description

Build a Lagrange polynomial interpolant of the marginal posterior, for plotting and for computing quantiles.

Usage

```
interpolate_marginal_posterior(
  margpost,
  method = c("auto", "polynomial", "spline")
)
```

Arguments

margpost The output of aghq::marginal_posterior. See the documentation for that

function.

method The method to use. Default is a k point polynomial interpolant using polynom::poly.calc().

This has been observed to result in unstable behaviour for larger numbers of quadrature points k, which is of course undesirable. If k > 3, you can set method = 'spline' to use splines::interpSpline() instead, which uses cubic B-Splines. These should always be better than a straight polynomial, except don't work when k < 4 which is why they aren't the default. If you try and set method = 'spline' with k < 4 it will be changed back to polynomial, with a warning.

Value

A function of theta which computes the log interpolated normalized marginal posterior.

See Also

Other summaries: compute_moment(), compute_pdf_and_cdf(), compute_quantiles(), marginal_posterior()

laplace_approximation Laplace Approximation

Description

Wrapper function to implement a Laplace approximation to the posterior. A Laplace approximation is AGHQ with k=1 quadrature points. However, the returned object is of a different class laplace, and a different summary method is given for it. It is especially useful for high-dimensional problems where the curse of dimensionality renders the use of k>1 quadrature points infeasible. The summary method reflects the fact that the user may be using this for a high-dimensional problem, and no plot method is given, because there isn't anything interesting to plot.

Usage

```
laplace_approximation(
   ff,
   startingvalue,
   optresults = NULL,
   control = default_control(),
   ...
)
```

Arguments

ff

A list with three elements:

- fn: function taking argument theta and returning a numeric value representing the log-posterior at theta
- gr: function taking argument theta and returning a numeric vector representing the gradient of the log-posterior at theta
- he: function taking argument theta and returning a numeric matrix representing the hessian of the log-posterior at theta

The user may wish to use numDeriv::grad and/or numDeriv::hessian to obtain these. Alternatively, the user may consider the TMB package. This list is deliberately formatted to match the output of TMB::MakeADFun.

startingvalue

Value to start the optimization. ff\$fn(startingvalue), ff\$gr(startingvalue), and ff\$he(startingvalue) must all return appropriate values without error.

optresults

Optional. A list of the results of the optimization of the log posterior, formatted according to the output of aghq::optimize_theta. The aghq::aghq function handles the optimization for you; passing this list overrides this, and is useful for when you know your optimization is too difficult to be handled by general-purpose software. See the software paper for several examples of this. If you're unsure whether this option is needed for your problem then it probably is not.

control

A list with elements

- method: optimization method to use:
 - 'sparse_trust' (default): trustOptim::trust.optim with method = 'sparse'
 - 'SR1' (default): trustOptim::trust.optim with method = 'SR1'
 - 'trust': trust::trust
 - 'BFGS': optim(...,method = "BFGS")

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Default is 'sparse_trust'.

• optcontrol: optional: a list of control parameters to pass to the internal optimizer you chose. The aghq package uses sensible defaults.

Additional arguments to be passed to ff\$fn, ff\$gr, and ff\$he.

Value

An object of class laplace with summary and plot methods. This is simply a list with elements lognormconst containing the log of the approximate normalizing constant, and optresults containing the optimization results formatted the same way as optimize_theta and aghq.

See Also

```
Other quadrature: aghq(), get_log_normconst(), marginal_laplace_tmb(), marginal_laplace(), normalize_logpost(), optimize_theta(), plot.aghq(), print.aghqsummary(), print.aghq(), print.laplacesummary(), print.laplace(), print.marginallaplacesummary(), summary.aghq(), summary.laplace(), summary.marginallaplace()
```

```
logfteta2d <- function(eta,y) {</pre>
  # eta is now (eta1,eta2)
  # y is now (y1,y2)
  n <- length(y)</pre>
  n1 <- ceiling(n/2)</pre>
  n2 \leftarrow floor(n/2)
  y1 <- y[1:n1]
  y2 \leftarrow y[(n1+1):(n1+n2)]
  eta1 <- eta[1]
  eta2 <- eta[2]
  sum(y1) * eta1 - (length(y1) + 1) * exp(eta1) - sum(lgamma(y1+1)) + eta1 +
    sum(y2) * eta2 - (length(y2) + 1) * exp(eta2) - sum(lgamma(y2+1)) + eta2
set.seed(84343124)
n1 <- 5
n2 <- 5
n < - n1+n2
y1 <- rpois(n1,5)
y2 \leftarrow rpois(n2,5)
objfunc2d <- function(x) logfteta2d(x,c(y1,y2))
funlist2d <- list(</pre>
  fn = objfunc2d,
  gr = function(x) numDeriv::grad(objfunc2d,x),
  he = function(x) numDeriv::hessian(objfunc2d,x)
thequadrature <- aghq(funlist2d,3,c(0,0))
```

18 marginal_laplace

Description

Implement the marginal Laplace approximation of Tierney and Kadane (1986) for finding the marginal posterior (theta | Y) from an unnormalized joint posterior (W, theta, Y) where W is high dimensional and theta is low dimensional. See the AGHQ software paper for a detailed example, or Stringer et. al. (2020).

Usage

```
marginal_laplace(
    ff,
    k,
    startingvalue,
    optresults = NULL,
    control = default_control_marglaplace(),
    ...
)
```

Arguments

ff

A function list similar to that required by aghq. However, each function now takes arguments W and theta. Explicitly, this is a list containing elements:

- fn: function taking arguments W and theta and returning a numeric value representing the log-joint posterior at W, theta
- gr: function taking arguments W and theta and returning a numeric vector representing the gradient with respect to W of the log-joint posterior at W, theta
- he: function taking arguments W and theta and returning a numeric matrix representing the hessian with respect to W of the log-joint posterior at W, theta

k

Integer, the number of quadrature points to use. I suggest at least 3. k = 1 corresponds to a Laplace approximation.

startingvalue

A list with elements W and theta, which are numeric vectors to start the optimizations for each variable. If you're using this method then the log-joint posterior should be concave and these optimizations should not be sensitive to starting values.

optresults

Optional. A list of the results of the optimization of the log posterior, formatted according to the output of aghq::optimize_theta. The aghq::aghq function handles the optimization for you; passing this list overrides this, and is useful for when you know your optimization is too difficult to be handled by general-purpose software. See the software paper for several examples of this. If you're unsure whether this option is needed for your problem then it probably is not.

control

A list with elements

- method: optimization method to use for the theta optimization:
 - 'sparse_trust' (default): trustOptim::trust.optim
 - 'sparse': trust::trust
 - 'BFGS': optim(..., method = "BFGS")
- inner_method: optimization method to use for the W optimization; same options as for method

Default inner_method is 'sparse_trust' and default method is 'BFGS'.

Additional arguments to be passed to ff\$fn, ff\$gr, and ff\$he.

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Value

If k > 1, an object of class marginallaplace, which includes the result of calling aghq::aghq on the Laplace approximation of (theta|Y), See software paper for full details. If k = 1, an object of class laplace which is the result of calling aghq::laplace_approximation on the Laplace approximation of (theta|Y).

See Also

```
Other quadrature: aghq(), get_log_normconst(), laplace_approximation(), marginal_laplace_tmb(), normalize_logpost(), optimize_theta(), plot.aghq(), print.aghqsummary(), print.aghq(), print.laplacesummary(), print.laplace(), print.marginallaplacesummary(), summary.aghq(), summary.laplace(), summary.marginallaplace()
```

```
logfteta2d <- function(eta,y) {</pre>
  # eta is now (eta1,eta2)
  # y is now (y1,y2)
  n <- length(y)</pre>
  n1 <- ceiling(n/2)</pre>
  n2 \leftarrow floor(n/2)
  y1 <- y[1:n1]
  y2 \leftarrow y[(n1+1):(n1+n2)]
  eta1 <- eta[1]
  eta2 <- eta[2]
  sum(y1) * eta1 - (length(y1) + 1) * exp(eta1) - sum(lgamma(y1+1)) + eta1 +
    sum(y2) * eta2 - (length(y2) + 1) * exp(eta2) - sum(lgamma(y2+1)) + eta2
set.seed(84343124)
n1 <- 5
n2 <- 5
n < - n1+n2
y1 <- rpois(n1,5)
y2 \leftarrow rpois(n2,5)
objfunc2d <- function(x) logfteta2d(x,c(y1,y2))
objfunc2dmarg <- function(W,theta) objfunc2d(c(W,theta))</pre>
objfunc2dmarggr <- function(W,theta) {</pre>
  fn <- function(W) objfunc2dmarg(W,theta)</pre>
  numDeriv::grad(fn,W)
objfunc2dmarghe <- function(W,theta) {</pre>
  fn <- function(W) objfunc2dmarg(W,theta)</pre>
  numDeriv::hessian(fn,W)
funlist2dmarg <- list(</pre>
  fn = objfunc2dmarg,
  gr = objfunc2dmarggr,
  he = objfunc2dmarghe
```

Description

Implement the algorithm from aghq::marginal_laplace(), but making use of TMB's automatic Laplace approximation. This function takes a function list from TMB::MakeADFun() with a nonempty set of random parameters, in which the fn and gr are the unnormalized marginal Laplace approximation and its gradient. It then calls aghq::aghq() and formats the resulting object so that its contents and class match the output of aghq::marginal_laplace() and are hence suitable for post-processing with summary, aghq::sample_marginal(), and so on.

Usage

```
marginal_laplace_tmb(
    ff,
    k,
    startingvalue,
    optresults = NULL,
    basegrid = NULL,
    control = default_control_tmb(),
    ...
)
```

Arguments

ff

The output of calling TMB::MakeADFun() with random set to a non-empty subset of the parameters. **VERY IMPORTANT**: TMB's automatic Laplace approximation requires you to write your template implementing the **negated** log-posterior. Therefore, this list that you input here will contain components fn, gr and he that implement the **negated** log-posterior and its derivatives. This is **opposite** to every other comparable function in the aghq package, and is done here to emphasize compatibility with TMB.

k

Integer, the number of quadrature points to use. I suggest at least 3. k = 1 corresponds to a Laplace approximation.

startingvalue

Value to start the optimization. ff\$fn(startingvalue), ff\$gr(startingvalue), and ff\$he(startingvalue) must all return appropriate values without error.

optresults

Optional. A list of the results of the optimization of the log posterior, formatted according to the output of aghq::optimize_theta. The aghq::aghq function handles the optimization for you; passing this list overrides this, and is useful for when you know your optimization is too difficult to be handled by general-purpose software. See the software paper for several examples of this. If you're unsure whether this option is needed for your problem then it probably is not.

basegrid

Optional. Provide an object of class NIGrid from the mvQuad package, representing the base quadrature rule that will be adapted. This is only for users who want more complete control over the quadrature, and is not necessary if you are fine with the default option which basically corresponds to mvQuad::createNIGrid(length(theta))

Note: the mvQuad functions used within aghq operate on grids in memory, so

your basegrid object will be changed after you run aghq.

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control

A list of control parameters. See ?default_control for details. Valid options are:

• method: optimization method to use for the theta optimization:

```
- 'sparse_trust' (default): trustOptim::trust.optim
```

- 'sparse': trust::trust

- 'BFGS': optim(...,method = "BFGS")

- inner_method: optimization method to use for the W optimization; same options as for method. Default inner_method is 'sparse_trust' and default method is 'BFGS'.
- negate: default TRUE. See ?default_control_tmb. Assumes that your TMB function template computes the **negated** log-posterior, which it must if you're using TMB's automatic Laplace approximation, which you must be if you're using this function!

.

Additional arguments to be passed to ff\$fn, ff\$gr, and ff\$he.

Details

Because TMB does not yet have the Hessian of the log marginal Laplace approximation implemented, a numerically-differentiated jacobian of the gradient is used via numDeriv::jacobian(). You can turn this off (using ff\$he() instead, which you'll have to modify yourself) using default_control_tmb(numhessian = FALSE).

Value

If k > 1, an object of class marginallaplace (and inheriting from class aghq) of the same structure as that returned by aghq::marginal_laplace(), with plot and summary methods, and suitable for input into aghq::sample_marginal() for drawing posterior samples.

See Also

Other quadrature: aghq(), get_log_normconst(), laplace_approximation(), marginal_laplace(), normalize_logpost(), optimize_theta(), plot.aghq(), print.aghqsummary(), print.aghq(), print.laplacesummary(), print.laplace(), print.marginallaplacesummary(), summary.aghq(), summary.laplace(), summary.marginallaplace()

marginal_posterior

Marginal Posteriors

Description

Compute the marginal posterior for a given parameter using AGHQ. This function is mostly called within aghq().

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Usage

```
marginal_posterior(
  optresults,
  k,
  j,
  basegrid = NULL,
  ndConstruction = "product"
)
```

Arguments

optresults	The results of calling aghq::optimize_theta(): see return value of that function.
k	Integer, the number of quadrature points to use. I suggest at least 3. $k = 1$ corresponds to a Laplace approximation.
j	Integer between 1 and the dimension of the parameter space. Which index of the parameter vector to compute the marginal posterior for.
basegrid	Optional. Provide an object of class NIGrid from the mvQuad package, representing the base quadrature rule that will be adapted. This is only for users who want more complete control over the quadrature, and is not necessary if you are fine with the default option which basically corresponds to mvQuad::createNIGrid(length(theta))
ndConstruction	Create a multivariate grid using a product or sparse construction? Passed directly to mvQuad::createNIGrid(), see that function for further details. Note that the use of sparse grids within aghq is currently experimental and not supported by tests. In particular, calculation of marginal posteriors is known to fail currently.

Value

a data.frame containing the normalized log marginal posterior for theta_j evaluated at the original quadrature points. Has columns "thetaj", "logpost_normalized", "weights", where j is the j you specified.

See Also

Other summaries: compute_moment(), compute_pdf_and_cdf(), compute_quantiles(), interpolate_marginal_pdf_and_cdf(), interpolate_margi

```
## A 2d example ##
logfteta2d <- function(eta,y) {
    # eta is now (eta1,eta2)
    # y is now (y1,y2)
    n <- length(y)
    n1 <- ceiling(n/2)
    n2 <- floor(n/2)
    y1 <- y[1:n1]
    y2 <- y[(n1+1):(n1+n2)]
    eta1 <- eta[1]
    eta2 <- eta[2]
    sum(y1) * eta1 - (length(y1) + 1) * exp(eta1) - sum(lgamma(y1+1)) + eta1 +
        sum(y2) * eta2 - (length(y2) + 1) * exp(eta2) - sum(lgamma(y2+1)) + eta2
}
set.seed(84343124)</pre>
```

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```
n1 <- 5
n2 <- 5
n <- n1+n2
y1 <- rpois(n1,5)
y2 \leftarrow rpois(n2,5)
objfunc2d <- function(x) logfteta2d(x,c(y1,y2))
funlist2d <- list(</pre>
  fn = objfunc2d,
  gr = function(x) numDeriv::grad(objfunc2d,x),
  he = function(x) numDeriv::hessian(objfunc2d,x)
opt_sparsetrust_2d <- optimize_theta(funlist2d,c(1.5,1.5))</pre>
# Now actually do the marginal posteriors
marginal_posterior(opt_sparsetrust_2d,3,1)
marginal_posterior(opt_sparsetrust_2d,3,2)
marginal_posterior(opt_sparsetrust_2d,7,2)
```

normalize_logpost

Normalize the joint posterior using AGHQ

Description

This function takes in the optimization results from aghq::optimize_theta() and returns a list with the quadrature points, weights, and normalization information. Like aghq::optimize_theta(), this is designed for use only within aghq::aghq, but is exported for debugging and documented in case you want to modify it somehow, or something.

Usage

```
normalize_logpost(
  optresults,
 k,
 whichfirst = 1,
 basegrid = NULL,
 ndConstruction = "product",
```

Arguments

optresults The results of calling aghq::optimize_theta(): see return value of that func-

Integer, the number of quadrature points to use. I suggest at least 3. k = 1k

corresponds to a Laplace approximation.

whichfirst Integer between 1 and the dimension of the parameter space, default 1. The user shouldn't have to worry about this: it's used internally to re-order the parameter vector before doing the quadrature, which is useful when calculating marginal posteriors.

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Optional. Provide an object of class NIGrid from the mvQuad package, representing the base quadrature rule that will be adapted. This is only for users who want more complete control over the quadrature, and is not necessary if you are fine with the default option which basically corresponds to mvQuad::createNIGrid(length(theta)

ndConstruction Create a multivariate grid using a product or sparse construction? Passed directly to mvQuad::createNIGrid(), see that function for further details. Note that the use of sparse grids within aghq is currently **experimental** and not supported by tests. In particular, calculation of marginal posteriors is known to fail currently.

.. Additional arguments to be passed to optresults\$ff, see ?optimize_theta.

Value

If k > 1, a list with elements:

- nodesandweights: a dataframe containing the nodes and weights for the adaptive quadrature rule, with the un-normalized and normalized log posterior evaluated at the nodes.
- thegrid: a NIGrid object from the mvQuad package, see ?mvQuad::createNIGrid.
- lognormconst: the actual result of the quadrature: the log of the normalizing constant of the posterior.

If k = 1, then the method returns a numeric value representing the log of the normalizing constant computed using a Laplace approximation.

See Also

```
Other quadrature: aghq(), get_log_normconst(), laplace_approximation(), marginal_laplace_tmb(), marginal_laplace(), optimize_theta(), plot.aghq(), print.aghqsummary(), print.aghq(), print.laplacesummary(), print.laplace(), print.marginallaplacesummary(), summary.aghq(), summary.laplace(), summary.marginallaplace()
```

```
# Same setup as optimize_theta
logfteta <- function(eta,y) {</pre>
  sum(y) * eta - (length(y) + 1) * exp(eta) - sum(lgamma(y+1)) + eta
}
set.seed(84343124)
y \leftarrow rpois(10,5) \# Mode should be sum(y) / (10 + 1)
truemode <- \log((sum(y) + 1)/(length(y) + 1))
objfunc <- function(x) logfteta(x,y)
funlist <- list(</pre>
  fn = objfunc,
  gr = function(x) numDeriv::grad(objfunc,x),
 he = function(x) numDeriv::hessian(objfunc,x)
opt_sparsetrust <- optimize_theta(funlist,1.5)</pre>
opt_trust <- optimize_theta(funlist,1.5,control = default_control(method = "trust"))</pre>
opt_bfgs <- optimize_theta(funlist,1.5,control = default_control(method = "BFGS"))</pre>
# Quadrature with 3, 5, and 7 points using sparse trust region optimization:
norm_sparse_3 <- normalize_logpost(opt_sparsetrust,3,1)</pre>
norm_sparse_5 <- normalize_logpost(opt_sparsetrust,5,1)</pre>
norm_sparse_7 <- normalize_logpost(opt_sparsetrust,7,1)</pre>
# Quadrature with 3, 5, and 7 points using dense trust region optimization:
```

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```
norm_trust_3 <- normalize_logpost(opt_trust,3,1)
norm_trust_5 <- normalize_logpost(opt_trust,5,1)
norm_trust_7 <- normalize_logpost(opt_trust,7,1)

# Quadrature with 3, 5, and 7 points using BFGS optimization:
norm_bfgs_3 <- normalize_logpost(opt_bfgs,3,1)
norm_bfgs_5 <- normalize_logpost(opt_bfgs,5,1)
norm_bfgs_7 <- normalize_logpost(opt_bfgs,7,1)</pre>
```

optimize_theta

Obtain function information necessary for performing quadrature

Description

This function computes the two pieces of information needed about the log posterior to do adaptive quadrature: the mode, and the hessian at the mode. It is designed for use within aghq::aghq, but is exported in case users need to debug the optimization process and documented in case users want to write their own optimizations.

Usage

```
optimize_theta(ff, startingvalue, control = default_control(), ...)
```

Arguments

ff

A list with three elements:

- fn: function taking argument theta and returning a numeric value representing the log-posterior at theta
- gr: function taking argument theta and returning a numeric vector representing the gradient of the log-posterior at theta
- he: function taking argument theta and returning a numeric matrix representing the hessian of the log-posterior at theta

The user may wish to use numDeriv::grad and/or numDeriv::hessian to obtain these. Alternatively, the user may consider the TMB package. This list is deliberately formatted to match the output of TMB::MakeADFun.

startingvalue

Value to start the optimization. ff\$fn(startingvalue), ff\$gr(startingvalue), and ff\$he(startingvalue) must all return appropriate values without error.

control

A list with elements

- method: optimization method to use:
 - 'sparse_trust' (default): trustOptim::trust.optim with method = 'sparse'
 - 'SR1' (default): trustOptim::trust.optim with method = 'SR1'
 - 'trust': trust::trust
 - 'BFGS': optim(...,method = "BFGS")

Default is 'sparse_trust'.

• optcontrol: optional: a list of control parameters to pass to the internal optimizer you chose. The aghq package uses sensible defaults.

... Additional arguments to be passed to ff\$fn, ff\$gr, and ff\$he.

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Value

A list with elements

- ff: the function list that was provided
- mode: the mode of the log posterior
- hessian: the hessian of the log posterior at the mode
- convergence: specific to the optimizer used, a message indicating whether it converged

See Also

```
Other quadrature: aghq(), get_log_normconst(), laplace_approximation(), marginal_laplace_tmb(), marginal_laplace(), normalize_logpost(), plot.aghq(), print.aghqsummary(), print.aghq(), print.laplacesummary(), print.laplace(), print.marginallaplacesummary(), summary.aghq(), summary.laplace(), summary.marginallaplace()
```

Examples

```
# Poisson/Exponential example
logfteta <- function(eta,y) {
   sum(y) * eta - (length(y) + 1) * exp(eta) - sum(lgamma(y+1)) + eta
}

y <- rpois(10,5) # Mode should be (sum(y) + 1) / (length(y) + 1)

objfunc <- function(x) logfteta(x,y)

funlist <- list(
   fn = objfunc,
   gr = function(x) numDeriv::grad(objfunc,x),
   he = function(x) numDeriv::hessian(objfunc,x)
)

optimize_theta(funlist,1.5)
optimize_theta(funlist,1.5,control = default_control(method = "trust"))
optimize_theta(funlist,1.5,control = default_control(method = "BFGS"))</pre>
```

plot.aghq

Plot method for AGHQ objects

Description

Plot the marginal pdf and cdf from an aghq object.

Usage

```
## S3 method for class 'aghq' plot(x, ...)
```

Arguments

```
x The return value of aghq::aghq.... not used.
```

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Value

Silently plots.

See Also

```
Other quadrature: aghq(), get_log_normconst(), laplace_approximation(), marginal_laplace_tmb(), marginal_laplace(), normalize_logpost(), optimize_theta(), print.aghqsummary(), print.aghq(), print.laplacesummary(), print.laplace(), print.marginallaplacesummary(), summary.aghq(), summary.laplace(), summary.marginallaplace()
```

Other quadrature: aghq(), get_log_normconst(), laplace_approximation(), marginal_laplace_tmb(), marginal_laplace(), normalize_logpost(), optimize_theta(), print.aghqsummary(), print.aghq(), print.laplacesummary(), print.laplace(), print.marginallaplacesummary(), summary.aghq(), summary.laplace(), summary.marginallaplace()

Examples

```
logfteta2d <- function(eta,y) {</pre>
  # eta is now (eta1,eta2)
  # y is now (y1,y2)
  n <- length(y)</pre>
  n1 <- ceiling(n/2)</pre>
  n2 \leftarrow floor(n/2)
  y1 <- y[1:n1]
  y2 \leftarrow y[(n1+1):(n1+n2)]
  eta1 <- eta[1]
  eta2 <- eta[2]
  sum(y1) * eta1 - (length(y1) + 1) * exp(eta1) - sum(lgamma(y1+1)) + eta1 +
    sum(y2) * eta2 - (length(y2) + 1) * exp(eta2) - sum(lgamma(y2+1)) + eta2
set.seed(84343124)
n1 <- 5
n2 <- 5
n < - n1+n2
y1 <- rpois(n1,5)
y2 \leftarrow rpois(n2,5)
objfunc2d <- function(x) logfteta2d(x,c(y1,y2))
funlist2d <- list(</pre>
  fn = objfunc2d,
  gr = function(x) numDeriv::grad(objfunc2d,x),
  he = function(x) numDeriv::hessian(objfunc2d,x)
thequadrature <- aghq(funlist2d,3,c(0,0))
plot(thequadrature)
```

print.aghq

Print method for AGHQ objects

Description

Pretty print the object—just gives some basic information and then suggests the user call summary(...).

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Usage

```
## S3 method for class 'aghq'
print(x, ...)
```

Arguments

x An object of class aghq.

... not used.

Value

Silently prints summary information.

See Also

```
Other quadrature: aghq(), get_log_normconst(), laplace_approximation(), marginal_laplace_tmb(), marginal_laplace(), normalize_logpost(), optimize_theta(), plot.aghq(), print.aghqsummary(), print.laplacesummary(), print.laplace(), print.marginallaplacesummary(), summary.aghq(), summary.laplace(), summary.marginallaplace()
```

```
logfteta2d <- function(eta,y) {</pre>
  # eta is now (eta1,eta2)
  \# y is now (y1,y2)
  n <- length(y)</pre>
  n1 <- ceiling(n/2)</pre>
  n2 \leftarrow floor(n/2)
  y1 <- y[1:n1]
  y2 \leftarrow y[(n1+1):(n1+n2)]
  eta1 <- eta[1]
  eta2 <- eta[2]
  sum(y1) * eta1 - (length(y1) + 1) * exp(eta1) - sum(lgamma(y1+1)) + eta1 +
    sum(y2) * eta2 - (length(y2) + 1) * exp(eta2) - sum(lgamma(y2+1)) + eta2
set.seed(84343124)
n1 <- 5
n2 <- 5
n <- n1+n2
y1 <- rpois(n1,5)
y2 \leftarrow rpois(n2,5)
objfunc2d <- function(x) logfteta2d(x,c(y1,y2))</pre>
funlist2d <- list(</pre>
  fn = objfunc2d,
  gr = function(x) numDeriv::grad(objfunc2d,x),
  he = function(x) numDeriv::hessian(objfunc2d,x)
)
thequadrature <- aghq(funlist2d,3,c(0,0))
thequadrature
```

print.aghqsummary 29

print.aghqsummary

Print method for AGHQ summary objects

Description

Print the summary of an aghq object. Almost always called by invoking summary(...) interactively in the console.

Usage

```
## S3 method for class 'aghqsummary' print(x, ...)
```

Arguments

x The result of calling summary(...) on an object of class aghq.... not used.

Value

Silently prints summary information.

See Also

```
Other quadrature: aghq(), get_log_normconst(), laplace_approximation(), marginal_laplace_tmb(), marginal_laplace(), normalize_logpost(), optimize_theta(), plot.aghq(), print.aghq(), print.laplacesummary(), print.laplace(), print.marginallaplacesummary(), summary.aghq(), summary.laplace(), summary.marginallaplace()

Other quadrature: aghq(), get_log_normconst(), laplace_approximation(), marginal_laplace_tmb(), marginal_laplace(), normalize_logpost(), optimize_theta(), plot.aghq(), print.aghq(), print.laplacesummary(), print.laplace(), print.marginallaplacesummary(), summary.aghq(), summary.laplace(), summary.marginallaplace()
```

```
logfteta2d <- function(eta,y) {</pre>
  # eta is now (eta1,eta2)
  # y is now (y1,y2)
  n <- length(y)</pre>
  n1 <- ceiling(n/2)</pre>
  n2 \leftarrow floor(n/2)
  y1 <- y[1:n1]
  y2 \leftarrow y[(n1+1):(n1+n2)]
  eta1 <- eta[1]
  eta2 <- eta[2]
  sum(y1) * eta1 - (length(y1) + 1) * exp(eta1) - sum(lgamma(y1+1)) + eta1 +
    sum(y2) \ * \ eta2 \ - \ (length(y2) \ + \ 1) \ * \ exp(eta2) \ - \ sum(lgamma(y2+1)) \ + \ eta2
}
set.seed(84343124)
n1 <- 5
n2 <- 5
n <- n1+n2
```

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```
y1 <- rpois(n1,5)
y2 <- rpois(n2,5)
objfunc2d <- function(x) logfteta2d(x,c(y1,y2))
funlist2d <- list(
    fn = objfunc2d,
    gr = function(x) numDeriv::grad(objfunc2d,x),
    he = function(x) numDeriv::hessian(objfunc2d,x)
)

thequadrature <- aghq(funlist2d,3,c(0,0))
# Summarize and automatically call its print() method when called interactively:
summary(thequadrature)</pre>
```

print.laplace

Print method for AGHQ objects

Description

Pretty print the object—just gives some basic information and then suggests the user call summary(...).

Usage

```
## S3 method for class 'laplace'
print(x, ...)
```

Arguments

```
x An object of class aghq.... not used.
```

Value

Silently prints summary information.

See Also

```
Other quadrature: aghq(), get_log_normconst(), laplace_approximation(), marginal_laplace_tmb(), marginal_laplace(), normalize_logpost(), optimize_theta(), plot.aghq(), print.aghqsummary(), print.aghq(), print.laplacesummary(), print.marginallaplacesummary(), summary.aghq(), summary.laplace(), summary.marginallaplace()
```

```
logfteta2d <- function(eta,y) {
    # eta is now (eta1,eta2)
    # y is now (y1,y2)
    n <- length(y)
    n1 <- ceiling(n/2)
    n2 <- floor(n/2)
    y1 <- y[1:n1]
    y2 <- y[(n1+1):(n1+n2)]
    eta1 <- eta[1]</pre>
```

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```
eta2 <- eta[2]
  sum(y1) * eta1 - (length(y1) + 1) * exp(eta1) - sum(lgamma(y1+1)) + eta1 +
    sum(y2) * eta2 - (length(y2) + 1) * exp(eta2) - sum(lgamma(y2+1)) + eta2
set.seed(84343124)
n1 <- 5
n2 <- 5
n <- n1+n2
y1 <- rpois(n1,5)</pre>
y2 \leftarrow rpois(n2,5)
objfunc2d <- function(x) logfteta2d(x,c(y1,y2))
funlist2d <- list(</pre>
  fn = objfunc2d,
  gr = function(x) numDeriv::grad(objfunc2d,x),
 he = function(x) numDeriv::hessian(objfunc2d,x)
)
thequadrature <- aghq(funlist2d,3,c(0,0))
thequadrature
```

print.laplacesummary Print method for laplacesummary objects

Description

Print the summary of an laplace object. Almost always called by invoking summary(...) interactively in the console.

Usage

```
## S3 method for class 'laplacesummary' print(x, ...)
```

Arguments

```
x The result of calling summary(...) on an object of class laplace.
... not used.
```

Value

Silently prints summary information.

See Also

```
Other quadrature: aghq(), get_log_normconst(), laplace_approximation(), marginal_laplace_tmb(), marginal_laplace(), normalize_logpost(), optimize_theta(), plot.aghq(), print.aghqsummary(), print.aghq(), print.laplace(), print.marginallaplacesummary(), summary.aghq(), summary.laplace(), summary.marginallaplace()
```

Other quadrature: aghq(), get_log_normconst(), laplace_approximation(), marginal_laplace_tmb(), marginal_laplace(), normalize_logpost(), optimize_theta(), plot.aghq(), print.aghqsummary(), print.aghq(), print.laplace(), print.marginallaplacesummary(), summary.aghq(), summary.laplace(), summary.marginallaplace()

Examples

```
logfteta2d <- function(eta,y) {</pre>
  # eta is now (eta1,eta2)
  # y is now (y1,y2)
  n <- length(y)</pre>
  n1 <- ceiling(n/2)</pre>
  n2 \leftarrow floor(n/2)
  y1 <- y[1:n1]
  y2 \leftarrow y[(n1+1):(n1+n2)]
  eta1 <- eta[1]
  eta2 <- eta[2]
  sum(y1) * eta1 - (length(y1) + 1) * exp(eta1) - sum(lgamma(y1+1)) + eta1 +
    sum(y2) * eta2 - (length(y2) + 1) * exp(eta2) - sum(lgamma(y2+1)) + eta2
}
set.seed(84343124)
n1 <- 5
n2 <- 5
n <- n1+n2
y1 <- rpois(n1,5)
y2 <- rpois(n2,5)
objfunc2d <- function(x) logfteta2d(x,c(y1,y2))
funlist2d <- list(</pre>
  fn = objfunc2d,
 gr = function(x) numDeriv::grad(objfunc2d,x),
 he = function(x) numDeriv::hessian(objfunc2d,x)
the laplace <- laplace_approximation(funlist2d,c(0,0))
# Summarize and automatically call its print() method when called interactively:
summary(thelaplace)
```

print.marginallaplacesummary

Summary statistics for models using marginal Laplace approximations

Description

The summary.marginallaplace calls summary.aghq, but also computes summary statistics of the random effects, by drawing from their approximate posterior using aghq::sample_marginal with the specified number of samples.

Usage

```
## S3 method for class 'marginallaplacesummary' print(x, ...)
```

Arguments

x Object of class marginallaplacesummary returned by calling summary on an object of class marginallaplace.

... not used.

Value

Nothing. Prints contents.

See Also

```
Other quadrature: aghq(), get_log_normconst(), laplace_approximation(), marginal_laplace_tmb(), marginal_laplace(), normalize_logpost(), optimize_theta(), plot.aghq(), print.aghqsummary(), print.aghq(), print.laplacesummary(), print.laplace(), summary.aghq(), summary.laplace(), summary.marginallaplace()
```

```
logfteta2d <- function(eta,y) {</pre>
  # eta is now (eta1,eta2)
  # y is now (y1,y2)
  n <- length(y)</pre>
  n1 <- ceiling(n/2)</pre>
  n2 \leftarrow floor(n/2)
  y1 <- y[1:n1]
  y2 \leftarrow y[(n1+1):(n1+n2)]
  eta1 <- eta[1]
  eta2 <- eta[2]
  sum(y1) * eta1 - (length(y1) + 1) * exp(eta1) - sum(lgamma(y1+1)) + eta1 +
    sum(y2) * eta2 - (length(y2) + 1) * exp(eta2) - sum(lgamma(y2+1)) + eta2
}
set.seed(84343124)
n1 <- 5
n2 <- 5
n <- n1+n2
y1 <- rpois(n1,5)
y2 \leftarrow rpois(n2,5)
objfunc2d <- function(x) logfteta2d(x,c(y1,y2))
objfunc2dmarg <- function(W,theta) objfunc2d(c(W,theta))
objfunc2dmarggr <- function(W,theta) {</pre>
  fn <- function(W) objfunc2dmarg(W,theta)</pre>
  numDeriv::grad(fn,W)
objfunc2dmarghe <- function(W,theta) {</pre>
  fn <- function(W) objfunc2dmarg(W,theta)</pre>
  numDeriv::hessian(fn,W)
}
funlist2dmarg <- list(</pre>
  fn = objfunc2dmarg,
  gr = objfunc2dmarggr,
  he = objfunc2dmarghe
)
themarginallaplace <- aghq::marginal_laplace(funlist2dmarg,3,list(W = 0,theta = 0))</pre>
summary(themarginallaplace)
```

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sample_marginal

Exact independent samples from an approximate posterior distribution

Description

Draws samples from an approximate marginal distribution for general posteriors approximated using aghq, or from the mixture-of-Gaussians approximation to the variables that were marginalized over in a marginal Laplace approximation fit using aghq::marginal_laplace or aghq::marginal_laplace_tmb.

Usage

```
sample_marginal(quad, ...)
## S3 method for class 'aghq'
sample_marginal(quad, M, transformation = NULL, interpolation = "auto", ...)
## S3 method for class 'marginallaplace'
sample_marginal(
  quad,
 Μ,
  transformation = NULL,
  interpolation = "auto",
  numcores = getOption("mc.cores", 1L),
)
```

Arguments

quad

Object from which to draw samples. An object inheriting from class marginallaplace (the result of running aghq::marginal_laplace or aghq::marginal_laplace_tmb), or an object inheriting from class aghq (the result of running aghq::aghq()). Can also provide a data.frame returned by aghq::compute_pdf_and_cdf in which case samples are returned for transparam if transformation is provided, and for paramif transformation = NULL.

Used to pass additional arguments.

М

Numeric, integer saying how many samples to draw

transformation Optional. A list containing function fromtheta() which accepts and returns numeric vectors, defining a parameter transformation for which you would like samples to be taken. See ?compute_pdf_and_cdf. Note that unlike there, where this operation is a bit more complicated, here all is done is samples are taken on the original scale and then transformation\$fromtheta() is called on them before returning.

interpolation

Which method to use for interpolating the marginal posteriors (and hence to draw samples using the inverse CDF method), 'auto' (choose for you), 'polynomial' or 'spline'? If k > 3 then the polynomial may be unstable and you should use the spline, but the spline doesn't work unless k > 3 so it's not the default. The default of 'auto' figures this out for you. See interpolate_marginal_posterior().

numcores

Integer, default getOption('mc.cores'). If greater than 1, the Cholesky decompositions of the Hessians are computed in parallel using parallel::mcapply, sample_marginal 35

for the Gaussian approximation involved for objects of class marginallaplace. This step is slow so may be sped up by parallelization, if the matrices are sparse (and hence the operation is just slow, but not memory-intensive). Uses the parallel package so is not available on Windows.

Details

For objects of class aghq or their marginal distribution components, sampling is done using the inverse CDF method, which is just compute_quantiles(quad\$marginals[[1]],runif(M)).

For marginal Laplace approximations (aghq::marginal_laplace()): this method samples from the posterior and returns a vector that is ordered the same as the "W" variables in your marginal Laplace approximation. See Algorithm 1 in Stringer et. al. (2021, https://arxiv.org/abs/2103.07425) for the algorithm; the details of sampling from a Gaussian are described in the reference(s) therein, which makes use of the (sparse) Cholesky factors. These are computed once for each quadrature point and stored.

For the marginal Laplace approximations where the "inner" model is handled entirely by TMB (aghq::marginal_laplace_tmb), the interface here is identical to above, with the order of the "W" vector being determined by TMB. See the names of ff\$env\$last.par, for example (where ff is your template obtained from a call to TMB::MakeADFun.

Value

If run on a marginal laplace object, a list containing elements:

- samps: d x M matrix where d = dim(W) and each column is a sample from pi(W|Y, theta)
- theta: M x S tibble where S = dim(theta) containing the value of theta for each sample
- thetasamples: A list of S numeric vectors each of length M where the jth element is a sample from pi(theta_{j}|Y). These are samples from the **marginals**, NOT the **joint**. Sampling from the joint is a much more difficult problem and how to do so in this context is an active area of research.

If run on an aghq object, then a list with just the thetasamples element. It still returns a list to maintain output consistency across inputs.

If, for some reason, you don't want to do the sampling from pi(theta|Y), you can manually set quad\$marginals = NULL. Note that this sampling is typically *very* fast and so I don't know why you would need to not do it but the option is there if you like.

If, again for some reason, you just want samples from one marginal distribution using inverse CDF, you can just do compute_quantiles(quad\$marginals[[1]],runif(M)).

```
logfteta2d <- function(eta,y) {
    # eta is now (eta1,eta2)
    # y is now (y1,y2)
    n <- length(y)
    n1 <- ceiling(n/2)
    n2 <- floor(n/2)
    y1 <- y[1:n1]
    y2 <- y[(n1+1):(n1+n2)]
    eta1 <- eta[1]
    eta2 <- eta[2]
    sum(y1) * eta1 - (length(y1) + 1) * exp(eta1) - sum(lgamma(y1+1)) + eta1 +
        sum(y2) * eta2 - (length(y2) + 1) * exp(eta2) - sum(lgamma(y2+1)) + eta2</pre>
```

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```
}
set.seed(84343124)
n1 <- 5
n2 <- 5
n <- n1+n2
y1 <- rpois(n1,5)
y2 <- rpois(n2,5)
objfunc2d <- function(x) logfteta2d(x,c(y1,y2))
objfunc2dmarg <- function(W,theta) objfunc2d(c(W,theta))</pre>
objfunc2dmarggr <- function(W,theta) {</pre>
  fn <- function(W) objfunc2dmarg(W,theta)</pre>
  numDeriv::grad(fn,W)
}
objfunc2dmarghe <- function(W,theta) {</pre>
  fn <- function(W) objfunc2dmarg(W,theta)</pre>
  numDeriv::hessian(fn,W)
}
funlist2dmarg <- list(</pre>
  fn = objfunc2dmarg,
  gr = objfunc2dmarggr,
  he = objfunc2dmarghe
```

summary.aghq

Summary statistics computed using AGHQ

Description

The summary aghq method computes means, standard deviations, and quantiles and the associated print method prints these along with diagnostic and other information about the quadrature.

Usage

```
## S3 method for class 'aghq'
summary(object, ...)
```

Arguments

```
object The return value from aghq::aghq.
... not used.
```

Value

A list of class aghqsummary, which has a print method. Elements:

- mode: the mode of the log posterior
- hessian: the hessian of the log posterior at the mode
- covariance: the inverse of the hessian of the log posterior at the mode
- cholesky: the upper cholesky trinagle of the hessian of the log posterior at the mode
- quadpoints: the number of quadrature points used in each dimension

summary.laplace 37

- dim: the dimension of the parameter space
- summarytable: a table containing the mean, median, mode, standard deviation and quantiles of each parameter, computed according to the posterior normalized using AGHQ

See Also

```
Other quadrature: aghq(), get_log_normconst(), laplace_approximation(), marginal_laplace_tmb(), marginal_laplace(), normalize_logpost(), optimize_theta(), plot.aghq(), print.aghqsummary(), print.aghq(), print.laplacesummary(), print.laplace(), print.marginallaplacesummary(), summary.laplace(), summary.marginallaplace()
```

Examples

```
logfteta2d <- function(eta,y) {</pre>
  # eta is now (eta1,eta2)
  # y is now (y1,y2)
  n <- length(y)</pre>
 n1 <- ceiling(n/2)</pre>
  n2 \leftarrow floor(n/2)
  y1 <- y[1:n1]
 y2 \leftarrow y[(n1+1):(n1+n2)]
  eta1 <- eta[1]
  eta2 <- eta[2]
  sum(y1) * eta1 - (length(y1) + 1) * exp(eta1) - sum(lgamma(y1+1)) + eta1 +
    sum(y2) * eta2 - (length(y2) + 1) * exp(eta2) - sum(lgamma(y2+1)) + eta2
}
set.seed(84343124)
n1 <- 5
n2 <- 5
n <- n1+n2
y1 <- rpois(n1,5)
y2 <- rpois(n2,5)
objfunc2d <- function(x) logfteta2d(x,c(y1,y2))
funlist2d <- list(</pre>
  fn = objfunc2d,
  gr = function(x) numDeriv::grad(objfunc2d,x),
 he = function(x) numDeriv::hessian(objfunc2d,x)
)
thequadrature <- aghq(funlist2d,3,c(0,0))
# Summarize and automatically call its print() method when called interactively:
summary(thequadrature)
# or, compute the summary and save for further processing:
ss <- summary(thequadrature)</pre>
str(ss)
```

summary.laplace

Summary method for Laplace Approximation objects

Description

Summary method for objects of class laplace. Similar to the method for objects of class aghq, but assumes the problem is high-dimensional and does not compute or print any large objects or summaries. See summary aghq for further information.

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Usage

```
## S3 method for class 'laplace'
summary(object, ...)
```

Arguments

```
object An object of class laplace. ... not used.
```

summary.aghq(), summary.marginallaplace()

Value

Silently prints summary information.

See Also

```
Other quadrature: aghq(), get_log_normconst(), laplace_approximation(), marginal_laplace_tmb(), marginal_laplace(), normalize_logpost(), optimize_theta(), plot.aghq(), print.aghqsummary(), print.aghq(), print.laplacesummary(), print.laplace(), print.marginallaplacesummary(), summary.aghq(), summary.marginallaplace()

Other quadrature: aghq(), get_log_normconst(), laplace_approximation(), marginal_laplace_tmb(), marginal_laplace(), normalize_logpost(), optimize_theta(), plot.aghq(), print.aghqsummary(), print.aghq(), print.laplacesummary(),
```

```
logfteta2d <- function(eta,y) {</pre>
  # eta is now (eta1,eta2)
  # y is now (y1,y2)
  n <- length(y)</pre>
  n1 <- ceiling(n/2)</pre>
  n2 \leftarrow floor(n/2)
  y1 <- y[1:n1]
  y2 \leftarrow y[(n1+1):(n1+n2)]
  eta1 <- eta[1]
  eta2 <- eta[2]
  sum(y1) * eta1 - (length(y1) + 1) * exp(eta1) - sum(lgamma(y1+1)) + eta1 +
    sum(y2) * eta2 - (length(y2) + 1) * exp(eta2) - sum(lgamma(y2+1)) + eta2
}
set.seed(84343124)
n1 <- 5
n2 <- 5
n <- n1+n2
y1 <- rpois(n1,5)</pre>
y2 \leftarrow rpois(n2,5)
objfunc2d <- function(x) logfteta2d(x,c(y1,y2))
funlist2d <- list(</pre>
  fn = objfunc2d,
  gr = function(x) numDeriv::grad(objfunc2d,x),
  he = function(x) numDeriv::hessian(objfunc2d,x)
the laplace \leftarrow laplace_approximation(funlist2d,c(0,0))
# Summarize and automatically call its print() method when called interactively:
summary(thelaplace)
```

```
summary.marginallaplace
```

Summary statistics for models using marginal Laplace approximations

Description

The summary.marginallaplace calls summary.aghq, but also computes summary statistics of the random effects, by drawing from their approximate posterior using aghq::sample_marginal with the specified number of samples.

Usage

```
## S3 method for class 'marginallaplace'
summary(object, M = 1000, max_print = 30, ...)
```

Arguments

object	Object inheriting from both classes aghq and marginallaplace, for example as returned by aghq::marginal_laplace or aghq::marginal_laplace_tmb.
М	Number of samples to use to compute summary statistics of the random effects. Default 1000. Lower runs faster, higher is more accurate.
max_print	Sometimes there are a lot of random effects. If there are more random effects than max_print, the random effects aren't summarized, and a note is printed to this effect. Default 30.
	not used.

Value

A list containing an object of class aghqsummary (see summary.aghq) plus the following objects:

See Also

```
Other quadrature: aghq(), get_log_normconst(), laplace_approximation(), marginal_laplace_tmb(), marginal_laplace(), normalize_logpost(), optimize_theta(), plot.aghq(), print.aghqsummary(), print.aghq(), print.laplacesummary(), print.laplace(), print.marginallaplacesummary(), summary.aghq(), summary.laplace()
```

```
logfteta2d <- function(eta,y) {
    # eta is now (eta1,eta2)
    # y is now (y1,y2)
    n <- length(y)
    n1 <- ceiling(n/2)
    n2 <- floor(n/2)
    y1 <- y[1:n1]
    y2 <- y[(n1+1):(n1+n2)]
    eta1 <- eta[1]
    eta2 <- eta[2]
    sum(y1) * eta1 - (length(y1) + 1) * exp(eta1) - sum(lgamma(y1+1)) + eta1 +</pre>
```

40 validate_control

```
sum(y2) * eta2 - (length(y2) + 1) * exp(eta2) - sum(lgamma(y2+1)) + eta2
}
set.seed(84343124)
n1 <- 5
n2 <- 5
n <- n1+n2
y1 <- rpois(n1,5)
y2 \leftarrow rpois(n2,5)
objfunc2d <- function(x) logfteta2d(x,c(y1,y2))
objfunc2dmarg <- function(W,theta) objfunc2d(c(W,theta))
objfunc2dmarggr <- function(W, theta) {</pre>
  fn <- function(W) objfunc2dmarg(W,theta)</pre>
  numDeriv::grad(fn,W)
objfunc2dmarghe <- function(W,theta) {</pre>
  fn <- function(W) objfunc2dmarg(W,theta)</pre>
  numDeriv::hessian(fn,W)
}
funlist2dmarg <- list(</pre>
  fn = objfunc2dmarg,
  gr = objfunc2dmarggr,
 he = objfunc2dmarghe
themarginallaplace <- aghq::marginal_laplace(funlist2dmarg,3,list(W = 0,theta = 0))</pre>
summary(themarginallaplace)
```

validate_control

Validate a control list

Description

This function checks that the names and value types for a supplied control list are valid and are unlikely to cause further errors within aghq and related functions. Users should not have to worry about this and should just use default_control() and related constructors.

Usage

```
validate_control(control, type = c("aghq", "marglaplace", "tmb"), ...)
```

Arguments

```
control A list.

type One of c('aghq', 'marglapace', 'tmb'). The type of control object to validate. Will basically validate against the arguments required by aghq, marginal_laplace, and marginal_laplace_tmb, respectively.

Not used.
```

Details

To users reading this: just use default_control(), default_control_marglaplace(), or default_control_tmb() as appropriate, to ensure that your control arguments are correct. This function just exists to provide more descriptive error messages in the event that an incompatible list is provided.

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Value

Logical, TRUE if the list of control arguments is valid, else FALSE.

```
validate_control(default_control())
validate_control(default_control_marglaplace(),type = "marglaplace")
validate_control(default_control_tmb(),type = "tmb")
```

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