Package 'TMB'

July 27, 2020

```
Type Package
Title Template Model Builder: A General Random Effect Tool Inspired by
     'ADMB'
Version 1.7.18
Date 2020-07-24
Maintainer Kasper Kristensen <kaskr@dtu.dk>
Author Kasper Kristensen [aut, cre, cph],
     Brad Bell [cph],
     Hans Skaug [ctb],
     Arni Magnusson [ctb],
     Casper Berg [ctb],
     Anders Nielsen [ctb],
     Martin Maechler [ctb],
     Theo Michelot [ctb],
     Mollie Brooks [ctb],
     Alex Forrence [ctb],
     Christoffer Moesgaard Albertsen [ctb],
     Cole Monnahan [ctb]
Copyright See the file COPYRIGHTS
Description With this tool, a user should be able to quickly implement
     complex random effect models through simple C++ templates. The package combines
     'CppAD' (C++ automatic differentiation), 'Eigen' (templated matrix-vector
     library) and 'CHOLMOD' (sparse matrix routines available from R) to obtain
     an efficient implementation of the applied Laplace approximation with exact
     derivatives. Key features are: Automatic sparseness detection, parallelism
     through 'BLAS' and parallel user templates.
License GPL-2
URL http://tmb-project.org
BugReports https://github.com/kaskr/adcomp/issues
Depends R (>= 3.0.0)
Imports graphics, methods, stats, utils, Matrix (>= 1.0-12)
LinkingTo Matrix, RcppEigen
```

Suggests numDeriv, parallel

RoxygenNote 6.0.1

NeedsCompilation yes

Repository CRAN

Index

Date/Publication 2020-07-27 05:10:33 UTC

R topics documented:

as.list.sdreport	3
benchmark	4
checkConsistency	5
compile	6
config	7
confint.tmbprofile	8
dynlib	8
FreeADFun	9
gdbsource	0
MakeADFun	1
newton	4
newtonOption	5
normalize	6
oneStepPredict	6
ppenmp	9
plot.tmbprofile 2	20
precompile 2	20
print.checkConsistency	1
print.sdreport	22
Rinterface	22
runExample	23
runSymbolicAnalysis	:3
sdreport 2	24
summary.checkConsistency	26
summary.sdreport	27
template	27
mbprofile	9
tmbroot	0

32

as.list.sdreport 3

	as.list.sdr	report Convert e	estimates to original list format.
--	-------------	------------------	------------------------------------

Description

Get estimated parameters or standard errors in the same shape as the original parameter list.

Usage

```
## S3 method for class 'sdreport'
as.list(x, what = "", report = FALSE, ...)
```

Arguments

```
    x Output from sdreport.
    what Select what to convert (Estimate / Std. Error).
    report Get AD reported variables rather than model parameters?
    ... Passed to summary.sdreport.
```

Details

This function converts the selected column what of summary(x, select = c("fixed","random"),...) to the same format as the original parameter list (re-ordered as the template parameter order). The argument what is partially matched among the column names of the summary table. The actual match is added as an attribute to the output.

Value

List of same shape as original parameter list.

Examples

```
## Not run:
example(sdreport)

## Estimates as a parameter list:
as.list(rep, "Est")

## Std Errors in the same list format:
as.list(rep, "Std")

## p-values in the same list format:
as.list(rep, "Pr", p.value=TRUE)

## AD reported variables as a list:
as.list(rep, "Estimate", report=TRUE)

## Bias corrected AD reported variables as a list:
```

4 benchmark

```
as.list(rep, "Est. (bias.correct)", report=TRUE)
## End(Not run)
```

benchmark

Benchmark parallel templates

Description

Benchmark parallel templates

Plot result of parallel benchmark

Usage

```
benchmark(obj, n = 10, expr = NULL, cores = NULL)
## S3 method for class 'parallelBenchmark'
plot(x, type = "b", ..., show = c("speedup",
    "time"), legendpos = "topleft")
```

Arguments

obj	Object from MakeADFun
n	Number of replicates to obtain reliable results.
expr	Optional expression to benchmark instead of default.
cores	Optional vector of cores.
X	Object to plot
type	Plot type
	Further plot arguments
show	Plot relative speedup or relative time?
legendpos	Position of legend

Details

By default this function will perform timings of the most critical parts of an AD model, specifically

- 1. Objective function of evaluated template.
- 2. Gradient of evaluated template.
- 3. Sparse hessian of evaluated template.
- 4. Cholesky factorization of sparse hessian.

(for pure fixed effect models only the first two). Expressions to time can be overwritten by the user (expr). A plot method is available for Parallel benchmarks.

checkConsistency 5

Examples

```
## Not run:
runExample("linreg_parallel",thisR=TRUE) ## Create obj
ben <- benchmark(obj,n=100,cores=1:4)
plot(ben)
ben <- benchmark(obj,n=10,cores=1:4,expr=expression(do.call("optim",obj)))
plot(ben)
## End(Not run)</pre>
```

checkConsistency

Check consistency and Laplace accuracy

Description

Check consistency of various parts of a TMB implementation. Requires that user has implemented simulation code for the data and optionally random effects. (*Beta version*; *may change without notice*)

Usage

```
checkConsistency(obj, par = NULL, hessian = FALSE, n = 100)
```

Arguments

obj Object from MakeADFun

par Parameter vector (θ) for simulation. If unspecified use the best encountered

parameter of the object.

hessian Calculate the hessian matrix for each replicate?

n Number of simulations

Details

This function checks that the simulation code of random effects and data is consistent with the implemented negative log-likelihood function. It also checks whether the approximate *marginal* score function is central indicating whether the Laplace approximation is suitable for parameter estimation.

Denote by u the random effects, θ the parameters and by x the data. The main assumption is that the user has implemented the joint negative log likelihood $f_{\theta}(u, x)$ satisfying

$$\int \int \exp(-f_{\theta}(u,x)) du dx = 1$$

It follows that the joint and marginal score functions are central:

1.
$$E_{u,x}\left[\nabla_{\theta}f_{\theta}(u,x)\right]=0$$

2.
$$E_x \left[\nabla_{\theta} - \log \left(\int \exp(-f_{\theta}(u, x)) du \right) \right] = 0$$

6 compile

For each replicate of u and x joint and marginal gradients are calculated. Appropriate centrality tests are carried out by summary.checkConsistency. An asymptotic χ^2 test is used to verify the first identity. Power of this test increases with the number of simulations n. The second identity holds approximately when replacing the marginal likelihood with its Laplace approximation. A formal test would thus fail eventually for large n. Rather, the gradient bias is transformed to parameter scale (using the estimated information matrix) to provide an estimate of parameter bias caused by the Laplace approximation.

Value

List with gradient simulations (joint and marginal)

See Also

```
summary.checkConsistency, print.checkConsistency
```

Examples

```
## Not run:
runExample("simple")
chk <- checkConsistency(obj)
chk
## Get more details
s <- summary(chk)
s$marginal$p.value ## Laplace exact for Gaussian models
## End(Not run)</pre>
```

compile

Compile a C++ template to DLL suitable for MakeADFun.

Description

Compile a C++ template into a shared object file. OpenMP flag is set if the template is detected to be parallel.

Usage

```
compile(file, flags = "", safebounds = TRUE, safeunload = TRUE,
  openmp = isParallelTemplate(file[1]), libtmb = TRUE, libinit = TRUE,
  tracesweep = FALSE, ...)
```

Arguments

file C++ file.

flags Character with compile flags.

safebounds Turn on preprocessor flag for bound checking?
safeunload Turn on preprocessor flag for safe DLL unloading?

config 7

openmp	Turn on openmp flag? Auto detected for parallel templates.
libtmb	Use precompiled TMB library if available (to speed up compilation)?
libinit	Turn on preprocessor flag to register native routines?
tracesweep	Turn on preprocessor flag to trace AD sweeps? (Silently disables libtmb)
	Passed as Makeconf variables

Details

TMB relies on R's built in functionality to create shared libraries independent of the platform. A template is compiled by compile("template.cpp"), which will call R's makefile with appropriate preprocessor flags. Compiler and compiler flags can be stored in a configuration file. In order of precedence either via the file pointed at by R_MAKEVARS_USER or the file ~/.R/Makevars if it exists. Additional configuration variables can be set with the flags and . . . arguments, which will override any previous selections.

See Also

precompile

config	Get or set internal configuration variables

Description

Get or set internal configuration variables of user's DLL.

Usage

```
config(..., DLL = getUserDLL())
```

Arguments

... Variables to setDLL Name of user's DLL. Auto-detected if missing.

Details

A model compiled with the TMB C++ library has several configuration variables set by default. The variables can be read and modified using this function. The meaning of the variables can be found in the Doxygen documentation.

Value

List with current configuration

8 dynlib

Examples

```
## Not run:
## Load library
dyn.load(dynlib("mymodel"))
## Read the current settings
config(DLL="mymodel")
## Reduce memory peak of a parallel model by creating tapes in serial
config(tape.parallel=0, DLL="mymodel")
obj <- MakeADFun(..., DLL="mymodel")
## End(Not run)</pre>
```

confint.tmbprofile

Profile based confidence intervals.

Description

Calculate confidence interval from a likelihood profile.

Usage

```
## S3 method for class 'tmbprofile'
confint(object, parm, level = 0.95, ...)
```

Arguments

object Output from tmbprofile.

parm Not used

level Confidence level.

... Not used

Value

Lower and upper limit as a matrix.

dynlib

Add dynlib extension

Description

Add the platform dependent dynlib extension. In order for examples to work across platforms DLLs should be loaded by dyn.load(dynlib("name")).

Usage

```
dynlib(name)
```

FreeADFun 9

Arguments

name

Library name without extension

Value

Character

FreeADFun

Free memory allocated on the C++ side by MakeADFun.

Description

Free memory allocated on the C++ side by MakeADFun.

Usage

FreeADFun(obj)

Arguments

obj

Object returned by MakeADFun

Details

An object returned by MakeADFun contains pointers to structures allocated on the C++ side. These are managed by R's garbage collector which for the most cases is sufficient. However, because the garbage collector is unware of the C++ object sizes, it may fail to release memory to the system as frequently as necessary. In such cases one can manually call FreeADFun(obj) to release the resources.

Memory management

- Garbage collection of an external pointer that is no longer needed (triggers corresponding finalizer).
- Explicit deallocation of external pointers using FreeADFun() (corresponding finalizers are untriggered but harmless).
- Unload/reload of the user's DLL deallocates all external pointers (corresponding finalizers are untriggered but harmless).

10 gdbsource

Note

This function is normally not needed.

Examples

```
runExample("simple", thisR = TRUE)
                                             ## Create 'obj'
FreeADFun(obj)
                                             ## Free external pointers
obj$fn()
                                             ## Re-allocate external pointers
```

gdbsource

Source R-script through gdb to get backtrace.

Description

Source R-script through gdb to get backtrace.

If gdbsource is run non-interactively (the default) only the relevant information will be printed.

Usage

```
gdbsource(file, interactive = FALSE)
## S3 method for class 'backtrace'
print(x, ...)
```

Arguments

file Your R script Run interactive gdb session? interactive Backtrace from gdbsource Х Not used

. . .

Details

This function is useful for debugging templates. If a script aborts e.g. due to an out-of-bound index operation it should be fast to locate the line that caused the problem by running gdbsource(file). Alternatively, If more detailed debugging is required, then gdbsource(file,TRUE) will provide the full backtrace followed by an interactive gdb session where the individual frames can be inspected. Note that templates should be compiled without optimization and with debug information in order to provide correct line numbers:

- On Linux/OS X use compile(cppfile, "-00 -g").
- On Windows use compile(cppfile, "-01 -g", DLLFLAGS="") (lower optimization level will cause errors).

Value

Object of class backtrace

MakeADFun 11

C++ template.	MakeADFun	Construct objective functions with derivatives based on a compiled C++ template.
---------------	-----------	--

Description

Construct objective functions with derivatives based on the users C++ template.

Usage

```
MakeADFun(data, parameters, map = list(), type = c("ADFun", "Fun",
   "ADGrad"[!is.null(random) || !is.null(profile)]), random = NULL,
   profile = NULL, random.start = expression(last.par.best[random]),
   hessian = FALSE, method = "BFGS", inner.method = "newton",
   inner.control = list(maxit = 1000), MCcontrol = list(doMC = FALSE, seed =
   123, n = 100), ADreport = FALSE, atomic = TRUE,
   LaplaceNonZeroGradient = FALSE, DLL = getUserDLL(),
   checkParameterOrder = TRUE, regexp = FALSE, silent = FALSE, ...)
```

Arguments

data	List of data objects (vectors, matrices, arrays, factors, sparse matrices) required by the user template (order does not matter and un-used components are al- lowed).
parameters	List of all parameter objects required by the user template (both random and fixed effects).
map	List defining how to optionally collect and fix parameters - see details.
type	Character vector defining which operation stacks are generated from the users template - see details.
random	Character vector defining the random effect parameters. See also regexp.
profile	Parameters to profile out of the likelihood (this subset will be appended to random with Laplace approximation disabled).
random.start	Expression defining the strategy for choosing random effect initial values as function of previous function evaluations - see details.
hessian	Calculate Hessian at optimum?
method	Outer optimization method.
inner.method	Inner optimization method (see function "newton").
inner.control	List controlling inner optimization.
MCcontrol	List controlling importance sampler (turned off by default).
ADreport	Calculate derivatives of macro ADREPORT(vector) instead of objective_function return value?
atomic	Allow tape to contain atomic functions?

12 MakeADFun

LaplaceNonZeroGradient

Allow Taylor expansion around non-stationary point?

DLL Name of shared object file compiled by user (without the conventional exten-

sion, '. so', '.dll', ...).

checkParameterOrder

Optional check for correct parameter order.

regexp Match random effects by regular expressions?

silent Disable all tracing information?

... Currently unused.

Details

A call to MakeADFun will return an object that, based on the users DLL code (specified through DLL), contains functions to calculate the objective function and its gradient. The object contains the following components:

- par A default parameter.
- fn The likelihood function.
- gr The gradient function.
- report A function to report all variables reported with the REPORT() macro in the user template.
- env Environment with access to all parts of the structure.

and is thus ready for a call to an R optimizer, such as nlminb or optim. Data (data) and parameters (parameters) are directly read by the user template via the macros beginning with DATA_ and PARAMETER_. The order of the PARAMETER_ macros defines the order of parameters in the final objective function. There are no restrictions on the order of random parameters, fixed parameters or data in the template.

Optionally, a simple mechanism for collecting and fixing parameters from R is available through the map argument. A map is a named list of factors with the following properties:

- names(map) is a subset of names(parameters).
- For a parameter "p" length(map\$p) equals length(parameters\$p).
- Parameter entries with NAs in the factor are fixed.
- Parameter entries with equal factor level are collected to a common value.

More advanced parameter mapping, such as collecting parameters between different vectors etc., must be implemented from the template.

Random effects are specified via the argument random: A component of the parameter list is marked as random if its name is matched by any of the characters of the vector random (Regular expression match is performed if regexp=TRUE). If some parameters are specified as random effects, these will be integrated out of the objective function via the Laplace approximation. In this situation the functions fn and gr automatically perform an optimization of random effects for each function evaluation. This is referred to as the 'inner optimization'. Strategies for choosing initial values of the inner optimization can be controlled via the argument random.start. The default is expression(last.par.best[random]) where last.par.best is an internal full

MakeADFun 13

parameter vector corresponding to the currently best likelihood. An alternative choice could be expression(last.par[random]) i.e. the random effect optimum of the most recent - not necessarily best - likelihood evaluation. Further control of the inner optimization can be obtained by the argument inner.control which is a list of control parameters for the inner optimizer newton. Depending of the inner optimization problem type the following settings are recommended:

- 1. Quasi-convex: smartsearch=TRUE (the default).
- 2. Strictly-convex: smartsearch=FALSE and maxit=20.
- 3. Quadratic: smartsearch=FALSE and maxit=1.

Technically, the user template is processed several times by inserting different types as template parameter, selected by argument type:

- "ADFun" Run through the template with AD-types and produce a stack of operations representing the objective function.
- "Fun" Run through the template with ordinary double-types.
- "ADGrad" Run through the template with nested AD-types and produce a stack of operations representing the objective function gradient.

Each of these are represented by external pointers to C++ structures available in the environment env.

Further objects in the environment env:

- validpar Function defining the valid parameter region (by default no restrictions). If an invalid parameter is inserted fn immediately return NaN.
- parList Function to get the full parameter vector of random and fixed effects in a convenient list format.
- random An index vector of random effect positions in the full parameter vector.
- last.par Full parameter of the latest likelihood evaluation.
- last.par.best Full parameter of the best likelihood evaluation.
- tracepar Trace every likelihood evaluation?
- tracemgc Trace maximum gradient component of every gradient evaluation?
- silent Pass 'silent=TRUE' to all try-calls ?

A high level of tracing information will be output by default when evaluating the objective function and gradient. This is useful while developing a model, but may eventually become annoying. Disable all tracing by passing silent=TRUE to the MakeADFun call.

Value

List with components (fn, gr, etc) suitable for calling an R optimizer, such as nlminb or optim.

Note

Do not rely upon the default arguments of any of the functions in the model object obj\$fn, obj\$gr, obj\$he, obj\$report. I.e. always use the explicit form obj\$fn(obj\$par) rather than obj\$fn().

14 newton

newton	Generalized newton optimizer.

Description

Generalized newton optimizer used for the inner optimization problem.

Usage

```
newton(par, fn, gr, he, trace = 1, maxit = 100, tol = 1e-08, alpha = 1,
   smartsearch = TRUE, mgcmax = 1e+60, super = TRUE, silent = TRUE,
   ustep = 1, power = 0.5, u0 = 1e-04, grad.tol = tol, step.tol = tol,
   tol10 = 0.001, env = environment(), ...)
```

Arguments

par	Initial parameter.
fn	Objective function.
gr	Gradient function.
he	Sparse hessian function.
trace	Print tracing information?
maxit	Maximum number of iterations.
tol	Convergence tolerance.
alpha	Newton stepsize in the fixed stepsize case.
smartsearch	Turn on adaptive stepsize algorithm for non-convex problems?
mgcmax	Refuse to optimize if the maximum gradient component is too steep.
super	Supernodal Cholesky?
silent	Be silent?
ustep	Adaptive stepsize initial guess between 0 and 1.
power	Parameter controlling adaptive stepsize.
u0	Parameter controlling adaptive stepsize.
grad.tol	Gradient convergence tolerance.
step.tol	Stepsize convergence tolerance.
tol10	Try to exit if last 10 iterations not improved more than this.
env	Environment for cached Cholesky factor.
	Currently unused.

newtonOption 15

Details

If smartsearch=FALSE this function performs an ordinary newton optimization on the function fn using an exact sparse hessian function. A fixed stepsize may be controlled by alpha so that the iterations are given by:

$$u_{n+1} = u_n - \alpha f''(u_n)^{-1} f'(u_n)$$

If smartsearch=TRUE the hessian is allowed to become negative definite preventing ordinary newton iterations. In this situation the newton iterations are performed on a modified objective function defined by adding a quadratic penalty around the expansion point u_0 :

$$f_t(u) = f(u) + \frac{t}{2} ||u - u_0||^2$$

This function's hessian (f''(u) + tI) is positive definite for t sufficiently large. The value t is updated at every iteration: If the hessian is positive definite t is decreased, otherwise increased. Detailed control of the update process can be obtained with the arguments ustep, power and u0.

Value

List with solution similar to optim output.

See Also

newtonOption

newtonOption

Set newton options for a model object.

Description

Inner-problem options can be set for a model object using this function.

Usage

```
newtonOption(obj, ...)
```

Arguments

obj Object from MakeADFun for which to change settings.

... Parameters for the newton optimizer to set.

Value

List of updated parameters.

16 oneStepPredict

norma	alize	Normalize process likelihood using the Laplace approximation.

Description

If the random effect likelihood contribution of a model has been implemented without proper normalization (i.e. lacks the normalizing constant), then this function can perform the adjustment automatically. In order for this to work, the model must include a flag that disables the data term so that the un-normalized random effect (negative log) density is returned from the model template. Automatic process normalization may be useful if either the normalizing constant is difficult to implement, or if its calulation involves so many operations that it becomes infeasible to include in the AD machinery.

Usage

```
normalize(obj, flag, value = 0)
```

Arguments

obj	Model object from MakeADFun without proper normalization of the random effect likelihood.
flag	Flag to disable the data term from the model.
value	Value of 'flag' that signifies to not include the data term.

Value

Modified model object that can be passed to an optimizer.

oneStepPredict Calculate one-step-ahead (OSA) residuals for a latent va	ariable model.
---	----------------

Description

Calculate one-step-ahead (OSA) residuals for a latent variable model. (*Beta version; may change without notice*)

Usage

```
oneStepPredict(obj, observation.name = NULL, data.term.indicator = NULL,
method = c("oneStepGaussianOffMode", "fullGaussian", "oneStepGeneric",
"oneStepGaussian", "cdf"), subset = NULL, conditional = NULL,
discrete = NULL, discreteSupport = NULL, range = c(-Inf, Inf),
seed = 123, parallel = FALSE, trace = TRUE, reverse = (method ==
"oneStepGaussianOffMode"), ...)
```

oneStepPredict 17

Arguments

obj Output from MakeADFun.

observation.name

Character naming the observation in the template.

data.term.indicator

Character naming an indicator data variable in the template (not required by all

methods - see details).

method Method to calculate OSA (see details).

subset Index vector of observations that will be added one by one during OSA. By

default 1:length(observations) (with conditional subtracted).

conditional Index vector of observations that are fixed during OSA. By default the empty

set.

discrete Are observations discrete? (assumed FALSE by default)

discreteSupport

Possible outcomes of discrete distribution (method="oneStepGeneric" only).

range Possible range of the observations.

seed Randomization seed (discrete case only). If NULL the RNG seed is untouched by

this routine.

parallel Run in parallel using the parallel package?

trace Trace progress?

reverse Do calculations in opposite order to improve stability? (currently enabled by

default for oneStepGaussianOffMode method only)

... Control parameters for OSA method

Details

Given a TMB latent variable model this function calculates OSA standardized residuals that can be used for goodness-of-fit assessment. The approach is based on a factorization of the joint distribution of the *observations* $X_1, ..., X_n$ into successive conditional distributions. Denote by

$$F_n(x_n) = P(X_n \le x_n | X_1 = x_1, ..., X_{n-1} = x_{n-1})$$

the one-step-ahead CDF, and by

$$p_n(x_n) = P(X_n = x_n | X_1 = x_1, ..., X_{n-1} = x_{n-1})$$

the corresponding point probabilities (zero for continuous distributions). In case of continuous observations the sequence

$$\Phi^{-1}(F_1(X_1)), ..., \Phi^{-1}(F_n(X_n))$$

will be iid standard normal. These are referred to as the OSA residuals. In case of discrete observations draw (unit) uniform variables $U_1, ..., U_n$ and construct the randomized OSA residuals

$$\Phi^{-1}(F_1(X_1)-U_1p_1(X_1))\;,...,\;\Phi^{-1}(F_n(X_n)-U_np_n(X_n))$$

These are also iid standard normal.

The user must specify one of the following methods to calculate the residuals:

18 oneStepPredict

method="fullGaussian" This method assumes that the joint distribution of data *and* random effects is Gaussian (or well approximated by a Gaussian). It does not require any changes to the user template. However, if used in conjunction with subset and/or conditional a data.term.indicator is required - see the next method.

method="oneStepGeneric" This method calculates the one-step conditional probability density as a ratio of Laplace approximations. The approximation is integrated (and re-normalized for improved accuracy) using 1D numerical quadrature to obtain the one-step CDF evaluated at each data point. The method works in the continuous case as well as the discrete case (discrete=TRUE).

It requires a specification of a data.term.indicator explained in the following. Suppose the template for the observations given the random effects (u) looks like

```
DATA_VECTOR(x);
...
nll -= dnorm(x(i), u(i), sd(i), true);
```

Then this template can be augmented with a data.term.indicator = "keep" by changing the template to

```
DATA_VECTOR(x);
DATA_VECTOR_INDICATOR(keep, x);
...
nll -= keep(i) * dnorm(x(i), u(i), sd(i), true);
...
```

The new data vector (keep) need not be passed from R. It automatically becomes a copy of x filled with ones.

- **method="oneStepGaussian"** This is a special case of the generic method where the one step conditional distribution is approximated by a Gaussian (and can therefore be handled more efficiently).
- **method="oneStepGaussianOffMode"** This is an approximation of the "oneStepGaussian" method that avoids locating the mode of the one-step conditional density.
- **method="cdf"** The generic method can be slow due to the many function evaluations used during the 1D integration (or summation in the discrete case). The present method can speed up this process but requires more changes to the user template. The above template must be expanded with information about how to calculate the negative log of the lower and upper CDF:

```
DATA_VECTOR(x);
DATA_VECTOR_INDICATOR(keep, x);
...
nll -= keep(i) * dnorm(x(i), u(i), 0.0, true);
nll -= keep.cdf_lower(i) * log( pnorm(x(i), u(i), 0.0) );
nll -= keep.cdf_upper(i) * log( 1.0 - pnorm(x(i), u(i), 0.0) );
```

The specialized members keep.cdf_lower and keep.cdf_upper automatically become copies of x filled with zeros.

openmp 19

Value

data. frame with OSA *standardized* residuals in column residual. Depending on the method the output may also include OSA expected observation in column mean.

Examples

openmp

Control number of openmp threads.

Description

Control number of openmp threads.

Usage

```
openmp(n = NULL)
```

Arguments

n

Requested number of threads, or NULL to just read the current value.

Value

Number of threads.

20 precompile

			_	
nl	\wedge t	tmbr	rnnt.	1 1 0
PLT	o.	LIIID	וט וכ	TTC

Plot likelihood profile.

Description

Plot (negative log) likelihood profile with confidence interval added.

Usage

```
## S3 method for class 'tmbprofile'
plot(x, type = "1", level = 0.95, ...)
```

Arguments

x Output from tmbprofile.

type Plot type.

level Add horizontal and vertical lines depicting this confidence level (NULL disables

the lines).

... Additional plot arguments.

precompile

Precompile the TMB library in order to speed up compilation of templates.

Description

Precompile the TMB library

Usage

```
precompile(all = TRUE, clean = FALSE, trace = TRUE, ...)
```

Arguments

all	Precompile all or	just the core	parts of TMB?

clean Remove precompiled libraries ?
trace Trace precompilation process ?

... Not used.

Details

Precompilation can be used to speed up compilation of templates. It is only necessary to run precompile() once, typically right after installation of TMB. The function *prepares* TMB for precompilation, while the actual pre-compilation takes place the first time you compile a model after running precompile().

Note that the precompilation requires write access to the TMB package folder. Three versions of the library will be prepared: Normal, parallel and a debugable version.

Precompilation works the same way on all platforms. The only known side-effect of precompilation is that it increases the file size of the generated binaries.

Examples

```
## Not run:
## Prepare precompilation
precompile()
## Perform precompilation by running a model
runExample(all = TRUE)
## End(Not run)
```

```
print.checkConsistency
```

Print output from checkConsistency

Description

Print diagnostics output from checkConsistency

Usage

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

Arguments

```
x Output from checkConsistency
```

... Not used

22 Rinterface

print.sdreport

Print brief model summary

Description

Print parameter estimates and give convergence diagnostic based on gradient and Hessian.

Usage

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

Arguments

x Output from sdreport

... Not used

Rinterface

Create minimal R-code corresponding to a cpp template.

Description

Create a skeleton of required R-code once the cpp template is ready.

Usage

```
Rinterface(file)
```

Arguments

file

cpp template file.

Examples

```
file <- system.file("examples/simple.cpp", package = "TMB")
Rinterface(file)</pre>
```

runExample 23

runExample	Run one of the test examples.	

Description

Compile and run a test example (runExample() shows all available examples).

Usage

```
runExample(name = NULL, all = FALSE, thisR = TRUE, clean = FALSE,
  exfolder = NULL, dontrun = FALSE, subarch = TRUE, ...)
```

Arguments

name	Character name of example.
all	Run all the test examples?
thisR	Run inside this R?
clean	Cleanup before compile?
exfolder	Alternative folder with examples.
dontrun	Build only (don't run) and remove temporary object files ?
subarch	Build in sub-architecture specific folder?
	Passed to compile.

 $run Symbolic Analysis \quad \textit{Run symbolic analysis on sparse Hessian}$

Description

Aggressively tries to reduce fill-in of sparse Cholesky factor by running a full suite of ordering algorithms. NOTE: requires a specialized installation of the package. More information is available at the package URL.

Usage

```
runSymbolicAnalysis(obj)
```

Arguments

obj Output from MakeADFun

24 sdreport

sdreport

General sdreport function.

Description

After optimization of an AD model, sdreport is used to calculate standard deviations of all model parameters, including non linear functions of random effects and parameters specified through the ADREPORT() macro from the user template.

Usage

```
sdreport(obj, par.fixed = NULL, hessian.fixed = NULL,
  getJointPrecision = FALSE, bias.correct = FALSE,
  bias.correct.control = list(sd = FALSE, split = NULL, nsplit = NULL),
  ignore.parm.uncertainty = FALSE, getReportCovariance = TRUE,
  skip.delta.method = FALSE)
```

Arguments

obj Object returned by MakeADFun

par.fixed Optional. Parameter estimate (will be known to obj when an optimization has

been carried out).

hessian.fixed Optional. Hessian wrt. parameters (will be calculated from obj if missing).

getJointPrecision

Optional. Return full joint precision matrix of random effects and parameters?

bias.correct logical indicating if bias correction should be applied

bias.correct.control

a list of bias correction options; currently $\operatorname{\mathsf{sd}}$, $\operatorname{\mathsf{split}}$ and $\operatorname{\mathsf{nsplit}}$ are used - $\operatorname{\mathsf{see}}$

details.

ignore.parm.uncertainty

Optional. Ignore estimation variance of parameters?

getReportCovariance

Get full covariance matrix of ADREPORTed variables?

skip.delta.method

Skip the delta method? (FALSE by default)

Details

First, the Hessian wrt. the parameter vector (θ) is calculated. The parameter covariance matrix is approximated by

$$V(\hat{\theta}) = -\nabla^2 l(\hat{\theta})^{-1}$$

where l denotes the log likelihood function (i.e. -obj\$fn). If ignore.parm.uncertainty=TRUE then the Hessian calculation is omitted and a zero-matrix is used in place of $V(\hat{\theta})$.

sdreport 25

For non-random effect models the standard delta-method is used to calculate the covariance matrix of transformed parameters. Let $\phi(\theta)$ denote some non-linear function of θ . Then

$$V(\phi(\hat{\theta})) \approx \nabla \phi V(\hat{\theta}) \nabla \phi'$$

The covariance matrix of reported variables $V(\phi(\hat{\theta}))$ is returned by default. This can cause high memory usage if many variables are ADREPORTed. Use getReportCovariance=FALSE to only return standard errors. In case standard deviations are not required one can completely skip the delta method using skip.delta.method=TRUE.

For random effect models a generalized delta-method is used. First the joint covariance of random effect and parameter estimation error is approximated by

$$V\begin{pmatrix} \hat{u} - u \\ \hat{\theta} - \theta \end{pmatrix} \approx \begin{pmatrix} H_{uu}^{-1} & 0 \\ 0 & 0 \end{pmatrix} + JV(\hat{\theta})J'$$

where H_{uu} denotes random effect block of the full joint Hessian of obj\$env\$f and J denotes the Jacobian of $\begin{pmatrix} \hat{u}(\theta) \\ \theta \end{pmatrix}$ wrt. θ . Here, the first term represents the expected conditional variance of the estimation error given the data and the second term represents the variance of the conditional mean of the estimation error given the data.

Now the delta method can be applied on a general non-linear function $\phi(u,\theta)$ of random effects u and parameters θ :

$$V\left(\phi(\hat{u}, \hat{\theta}) - \phi(u, \theta)\right) \approx \nabla \phi V\left(\frac{\hat{u} - u}{\hat{\theta} - \theta}\right) \nabla \phi'$$

The full joint covariance is not returned by default, because it may require large amounts of memory. It may be obtained by specifying getJointPrecision=TRUE, in which case $V\begin{pmatrix} \hat{u}-u\\ \hat{\theta}-\theta \end{pmatrix}^{-1}$ will be part of the output. This matrix must be manually inverted using solve(jointPrecision) in order to get the joint covariance matrix. Note, that the parameter order will follow the original order (i.e. obj\$env\$par).

Using $\phi(\hat{u}, \theta)$ as estimator of $\phi(u, \theta)$ may result in substantial bias. This may be the case if either ϕ is non-linear or if the distribution of u given x (data) is sufficiently non-symmetric. A generic correction is enabled with bias.correct=TRUE. It is based on the identity

$$E_{\theta}[\phi(u,\theta)|x] = \partial_{\varepsilon} \left(\log \int \exp(-f(u,\theta) + \varepsilon \phi(u,\theta)) \, du \right)_{|\varepsilon=0}$$

stating that the conditional expectation can be written as a marginal likelihood gradient wrt. a nuisance parameter ε . The marginal likelihood is replaced by its Laplace approximation.

If bias.correct.control\$sd=TRUE the variance of the estimator is calculated using

$$V_{\theta}[\phi(u,\theta)|x] = \partial_{\varepsilon}^{2} \left(\log \int \exp(-f(u,\theta) + \varepsilon \phi(u,\theta)) \ du \right)_{|\varepsilon=0}$$

A further correction is added to this variance to account for the effect of replacing θ by the MLE $\hat{\theta}$ (unless ignore.parm.uncertainty=TRUE).

Bias correction can be be performed in chunks in order to reduce memory usage or in order to only bias correct a subset of variables. First option is to pass a list of indices as bias.correct.control\$split.

E.g. a list list(1:2,3:4) calculates the first four ADREPORTed variables in two chunks. The internal function obj\$env\$ADreportIndex() gives an overview of the possible indices of ADREPORTed variables.

Second option is to pass the number of chunks as bias.correct.control\$nsplit in which case all ADREPORTed variables are bias corrected in the specified number of chunks. Also note that skip.delta.method may be necessary when bias correcting a large number of variables.

Value

Object of class sdreport

See Also

```
summary.sdreport, print.sdreport, as.list.sdreport
```

Examples

```
runExample("linreg_parallel", thisR = TRUE) ## Non-random effect example
sdreport(obj)
## End(Not run)
runExample("simple", thisR = TRUE)
                                             ## Random effect example
rep <- sdreport(obj)</pre>
summary(rep, "random")
                                             ## Only random effects
summary(rep, "fixed", p.value = TRUE)
                                             ## Only non-random effects
summary(rep, "report")
                                             ## Only report
## Bias correction
rep <- sdreport(obj, bias.correct = TRUE)</pre>
summary(rep, "report")
                                             ## Include bias correction
```

summary.checkConsistency

Summarize output from checkConsistency

Description

Summarize output from checkConsistency

Usage

```
## S3 method for class 'checkConsistency'
summary(object, na.rm = FALSE, ...)
```

Arguments

```
object Output from checkConsistency
na.rm Logical; Remove failed simulations?
Not used
```

summary.sdreport 27

Value

List of diagnostics

summary.sdreport

summary tables of model parameters

Description

Extract parameters, random effects and reported variables along with uncertainties and optionally Chi-square statistics. Bias corrected quantities are added as additional columns if available.

Usage

```
## S3 method for class 'sdreport'
summary(object, select = c("all", "fixed", "random",
    "report"), p.value = FALSE, ...)
```

Arguments

object Output from sdreport

select Parameter classes to select. Can be any subset of "fixed" $(\hat{\theta})$, "random" (\hat{u}) or

"report" $(\phi(\hat{u}, \hat{\theta}))$ using notation as sdreport.

p. value Add column with approximate p-values

... Not used

Value

matrix

template

Create cpp template to get started.

Description

Create a cpp template to get started.

Usage

```
template(file = NULL)
```

Arguments

file

Optional name of cpp file.

28 template

Details

This function generates a C++ template with a header and include statement. Here is a brief overview of the C++ syntax used to code the objective function. For a full reference see the Doxygen documentation (more information at the package URL).

Macros to read data and declare parameters:

Template Syntax	C++ type	R type
DATA_VECTOR(name)	vector <type></type>	vector
DATA_MATRIX(name)	matrix <type></type>	matrix
DATA_SCALAR(name)	Type	numeric(1)
DATA_INTEGER(name)	int	integer(1)
DATA_FACTOR(name)	vector <int></int>	factor
DATA_IVECTOR(name)	vector <int></int>	integer
DATA_SPARSE_MATRIX(name)	Eigen::SparseMatrix <type></type>	dgTMatrix
DATA_ARRAY(name)	array <type></type>	array
PARAMETER_MATRIX(name)	matrix <type></type>	matrix
PARAMETER_VECTOR(name)	vector <type></type>	vector
PARAMETER_ARRAY(name)	array <type></type>	array
PARAMETER(name)	Type	numeric(1)

Basic calculations:

Template Syntax	Explanation
REPORT(x)	Report x back to R
ADREPORT(x)	Report x back to R with derivatives
vector $<$ Type $>$ v(n1);	R equivalent of v=numeric(n1)
matrix <type> m(n1,n2);</type>	R equivalent of m=matrix(0,n1,n2)
array < Type > a(n1,n2,n3);	R equivalent of $a=array(0,c(n1,n2,n3))$
v+v,v-v,v*v,v/v	Pointwise binary operations
m*v	Matrix-vector multiply
a.col(i)	R equivalent of a[,,i]
a.col(i).col(j)	R equivalent of a[,j,i]
a(i,j,k)	R equivalent of a[i,j,k]
exp(v)	Pointwise math
m(i,j)	R equivalent of m[i,j]
v.sum()	R equivalent of sum(v)
m.transpose()	R equivalent of t(m)

Some distributions are available as C++ templates with syntax close to R's distributions:

Function header	Distribution
<pre>dnbinom2(x,mu,var,int give_log=0)</pre>	Negative binomial with mean and variance
<pre>dpois(x,lambda,int give_log=0)</pre>	Poisson distribution as in R
dlgamma(y,shape,scale,int give_log=0)	log-gamma distribution
<pre>dnorm(x,mean,sd,int give_log=0)</pre>	Normal distribution as in R

tmbprofile 29

Examples

template()

tmbprofile

Adaptive likelihood profiling.

Description

Calculate 1D likelihood profiles wrt. single parameters or more generally, wrt. arbitrary linear combinations of parameters (e.g. contrasts).

Usage

```
tmbprofile(obj, name, lincomb, h = 1e-04, ytol = 2, ystep = 0.1,
  maxit = ceiling(5 * ytol/ystep), parm.range = c(-Inf, Inf),
  slice = FALSE, trace = TRUE, ...)
```

Arguments

obj Object from MakeADFun that has been optimized.

name Name or index of a parameter to profile.

lincomb Optional linear combination of parameters to profile. By default a unit vector

corresponding to name.

h Initial adaptive stepsize on parameter axis.

ytol Adjusts the range of the likelihood values.

ystep Adjusts the resolution of the likelihood profile.

maxit Max number of iterations for adaptive algorithm.

parm. range Valid parameter range.

slice Do slicing rather than profiling?

trace Trace progress? (TRUE, or a numeric value of 1, gives basic tracing: numeric

values > 1 give more information)

... Unused

Details

Given a linear combination

$$t = \sum_{i=1}^{n} v_i \theta_i$$

of the parameter vector θ , this function calculates the likelihood profile of t. By default v is a unit vector determined from name. Alternatively the linear combination may be given directly (lincomb).

30 tmbroot

Value

data.frame with parameter and function values.

See Also

```
plot.tmbprofile,confint.tmbprofile
```

Examples

```
## Not run:
runExample("simple",thisR=TRUE)
## Parameter names for this model:
## beta beta logsdu logsd0

## Profile wrt. sigma0:
prof <- tmbprofile(obj,"logsd0")
plot(prof)
confint(prof)

## Profile the difference between the beta parameters (name is optional):
prof2 <- tmbprofile(obj,name="beta1 - beta2",lincomb = c(1,-1,0,0))
plot(prof2)
confint(prof2)

## End(Not run)</pre>
```

tmbroot

Compute likelihood profile confidence intervals of a TMB object by root-finding

Description

Compute likelihood profile confidence intervals of a TMB object by root-finding in contrast to tmbprofile, which tries to compute somewhat equally spaced values along the likelihood profile (which is useful for visualizing the shape of the likelihood surface), and then (via confint.tmbprofile) extracting a critical value by linear interpolation,

Usage

```
tmbroot(obj, name, target = 0.5 * qchisq(0.95, df = 1), lincomb,
  parm.range = c(NA, NA), sd.range = 7, trace = FALSE,
  continuation = FALSE)
```

Arguments

obj Object from MakeADFun that has been optimized.

name Name or index of a parameter to profile.

tmbroot 31

desired deviation from minimum log-likelihood. Default is set to retrieve the 95 target if the objective function is a negative log-likelihood function lincomb Optional linear combination of parameters to profile. By default a unit vector corresponding to name. parm.range lower and upper limits; if NA, a value will be guessed based on the parameter value and sd. range in the absence of explicit parm. range values, the range chosen will be the pasd.range rameter value plus or minus sd. range. May be specified as a two-element vector for different ranges below and above the parameter value. report information? trace continuation use continuation method, i.e. set starting parameters for non-focal parameters to solutions from previous fits?

Value

a two-element numeric vector containing the lower and upper limits (or NA if the target is not achieved in the range), with an attribute giving the total number of function iterations used

Examples

```
## Not run:
runExample("simple",thisR=TRUE)
logsd0.ci <- tmbroot(obj,"logsd0")
## End(Not run)</pre>
```

Index

```
as.list.sdreport, 3, 26
benchmark, 4
checkConsistency, 5, 21, 26
compile, 6, 23
config, 7
confint.tmbprofile, 8, 30
{\sf dynlib}, \textcolor{red}{8}
FreeADFun, 9
gdbsource, 10
MakeADFun, 11, 15
newton, 14, 15
newtonOption, 15, 15
normalize, 16
{\tt oneStepPredict}, \color{red} 16
openmp, 19
plot.parallelBenchmark (benchmark), 4
plot.tmbprofile, 20, 30
precompile, 7, 20
print.backtrace (gdbsource), 10
print.checkConsistency, 6, 21
print.sdreport, 22, 26
Rinterface, 22
runExample, 23
runSymbolicAnalysis, 23
sdreport, 3, 22, 24, 27
summary.checkConsistency, 6, 26
summary.sdreport, 3, 26, 27
template, 27
tmbprofile, 8, 20, 29, 30
tmbroot, 30
```