Package 'fmcmc'

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Title A friendly MCMC framework

```
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Description Provides a friendly (flexible) Markov Chain Monte Carlo (MCMC)
     framework for implementing Metropolis-Hastings algorithm in a modular way
     allowing users to specify automatic convergence checker, personalized
     transition kernels, and out-of-the-box multiple MCMC chains using
     parallel computing. Most of the methods implemented in this package can
     be found in Brooks et al. (2011, ISBN 9781420079425). Among the methods
     included, we have: Haario (2001) <doi:10.1007/s11222-011-9269-5>
     Adaptive Metropolis, Vihola (2012) <doi:10.1007/s11222-011-9269-5>
     Robust Adaptive Metropolis, and Thawornwattana et
     al. (2018) <doi:10.1214/17-BA1084> Mirror transition kernels.
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```

2 append_chains

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Contents

	check_initial	
	convergence-checker	
	cov_recursive	
	fmcmc	9
	fmcmc-deprecated	9
	kernel_adapt	10
	kernel_mirror	12
	kernel_new	
	kernel_normal	
	kernel_ram	
	kernel_unif	
	lifeexpect	
	MCMC	
	mcmc-loop	
	mcmc-output	
	new_progress_bar	
	plan_update_sequence	
	reflect on boundaries	
	Tenect_on_boundaries	30
Index		37

Description

Combines two or more MCMC runs into a single run. If runs have multiple chains, it will check that all have the same number of chains, and it will join chains using the rbind function.

Usage

```
append_chains(...)
```

Arguments

.. A list of mcmc or mcmc.list class objects.

Value

If mcmc.list, an object of class mcmc.list, otherwise, an object of class mcmc.

check_initial 3

Examples

```
# Appending two chains
data("lifeexpect")
logpost <- function(p) {</pre>
  sum(with(lifeexpect, dnorm(
    age - p[1] - smoke * p[2] - female * p[3],
    sd = p[4], log = TRUE)
  ))
}
# Using the RAM kernel
kern \leftarrow kernel_ram(lb = c(-100, -100, -100, .00001))
init <- c(</pre>
  avg_age = 70,
  smoke = 0,
  female = 0,
  sd
)
ans0 <- MCMC(initial = init, fun = logpost, nsteps = 1000, seed = 22, kernel = kern)
ans1 <- MCMC(initial = ans0, fun = logpost, nsteps = 2000, seed = 55, kernel = kern)
ans2 <- MCMC(initial = ans1, fun = logpost, nsteps = 2000, seed = 1155, kernel = kern)
ans_tot <- append_chains(ans0, ans1, ans2)</pre>
# Looking at the posterior distributions (see ?lifeexpect for info about
# the model). Only the trace
op \leftarrow par(mfrow = c(2,2))
for (i in 1:4)
  coda::traceplot(ans_tot[, i, drop=FALSE])
par(op)
```

check_initial

Checks the initial values of the MCMC

Description

This function is for internal use only.

Usage

```
check_initial(initial, nchains)
```

Arguments

```
initial Either a vector or matrix,.

nchains Integer scalar. Number of chains.
```

4 convergence-checker

Details

When initial is a vector, the values are recycled to form a matrix of size nchains * length(initial).

Value

A named matrix.

Examples

```
init <- c(.4, .1)
check_initial(init, 1)
check_initial(init, 2)

init <- matrix(1:9, ncol=3)
check_initial(init, 3)

# check_initial(init, 2) # Returns an error</pre>
```

convergence-checker

Convergence Monitoring

Description

Built-in set of functions to be used in companion with the argument conv_checker in MCMC. These functions are not intended to be used in a context other than the MCMC function.

The object LAST_CONV_CHECK is an environment that holds information regarding the convergence checker used. This information can be updated every time that the conv_checker function is called by MCMC using the functions convergence_data_set and convergence_msg_set. The function convergence_data_get is just a wrapper of get().

The msg member of LAST_CONV_CHECK is resetted before conv_checker is called.

Usage

```
LAST_CONV_CHECK

convergence_data_set(x)

convergence_data_get(x)

convergence_msg_set(msg = NA_character_)

convergence_msg_get()

convergence_gelman(freq = 1000L, threshold = 1.1, check_invariant = TRUE, ...)

convergence_geweke(
```

convergence-checker 5

```
freq = 1000L,
  threshold = 0.025,
  check_invariant = TRUE,
  ...
)

convergence_heildel(freq = 1000L, ..., check_invariant = TRUE)

convergence_auto(freq = 1000L)
```

Arguments

x In the case of convergence_data_set, a named list. For convergence_data_get,

a character vector.

msg Character scalar. Personalized message to print.

freq Integer scalar. Frequency of checking.

threshold Numeric value. A Gelman statistic below the threshold will return TRUE.

check_invariant

Logical. When TRUE the function only computes the Gelman diagnostic using

variables with greater than 1e-10 variance.

... Further arguments passed to the method.

Format

An object of class fmcmc_output_conv_check (inherits from environment) of length 1.

Details

convergence_gelman is a wrapper of coda::gelman.diag().

In the case of convergence_geweke, threshold sets the p-value for the null $H_0: Z=0$, i.e. equal means between the first and last chunks of the chain. See coda::geweke.diag. This implies that the higher the threshold, the lower the probability of stopping the chain.

In the case that the chain has more than one parameter, the algorithm will return true if and only if the test fails to reject the null for all the parameters.

For the convergence_heildel, see coda::heidel.diag for details.

The convergence_auto function is the default and is just a wrapper for convergence_gelman and convergence_geweke. This function returns a convergence checker that will be either of the other two depending on whether nchains in MCMC is greater than one—in which case it will use the Gelman test—or not—in which case it will use the Geweke test.

Value

A function passed to MCMC to check automatic convergence.

6 convergence-checker

Building a convergence checker

Convergence checkers are simply a function that receives as argument a matrix (or list of them) with sampled values, and returns a logical scalar with the value TRUE if the chain converged. An example of a personalized convergence checker is provided below. The frequency with which the check is performed is retrieved from the attribute "freq" from the convergence checker function, i.e., attr(..., "freq"). If missing, convergence will be checked halfway the number of steps in the chain, i.e., floor(nsteps/2).

Examples

```
# Example 1: Presonalized conv checker ------
# Dummy rule, if acceptance rate is near between .2 and .3.
convergence_example <- function(x) {</pre>
 arate <- 1 - coda::rejectionRate(x)</pre>
 all(
    abs(arate - .25) < .05
 )
}
# Tell fmcmc::MCMC what is the frequency
attr(convergence_example, "freq") <- 2e3
set.seed(223)
x <- rnorm(1000)
y < -x * 2 + rnorm(1000)
logpost <- function(p) {</pre>
 sum(dnorm(y, mean = x * p, log = TRUE))
}
ans <- MCMC(
 initial = 0, fun = logpost, nsteps = 5e4,
 kernel= kernel_ram(),
 conv_checker = convergence_example
# Example 2: Adding information ------
# Here we do two things: Save a value and set a message for the user
convergence_example_with_info <- structure(function(x) {</pre>
 arate <- 1 - coda::rejectionRate(x)</pre>
 # Saving a value
 if (!exists("arates", envir = LAST_CONV_CHECK, inherits = FALSE)) {
   convergence_data_set(list(arates = arate))
 } else {
   convergence_data_set(list(
     arates = rbind(convergence_data_get("arates"), arate)
   ))
 }
 # Setting up the message
 convergence_msg_set(
    sprintf("Current Avg. Accept. Rate: %.2f", mean(arate))
```

cov_recursive 7

```
all(
   abs(arate - .25) < .05
)
}, freq = 2000)

ans <- MCMC(
  initial = 0, fun = logpost, nsteps = 5e4,
  kernel= kernel_ram(),
  conv_checker = convergence_example_with_info,
  seed = 112,
  progress = FALSE
)</pre>
```

cov_recursive

Recursive algorithms for computing variance and mean

Description

These algorithms are used in kernel_adapt() to simplify variance-covariance recalculation at every step of the algorithm.

Usage

```
cov_recursive(
   X_t,
   Cov_t,
   Mean_t_prev,
   t.,
   Mean_t = NULL,
   eps = 0,
   Sd = 1,
   Ik = diag(ncol(Cov_t))
)
mean_recursive(X_t, Mean_t_prev, t.)
```

Arguments

8 cov_recursive

Details

The variance covariance algorithm was described in Haario, Saksman and Tamminen (2002).

References

Haario, H., Saksman, E., & Tamminen, J. (2001). An adaptive Metropolis algorithm. Bernoulli, 7(2), 223–242. https://projecteuclid.org/euclid.bj/1080222083

Examples

```
# Generating random data (only four points to see the difference)
set.seed(1231)
n <- 3
X \leftarrow matrix(rnorm(n*4), ncol = 4)
# These two should be equal
mean_recursive(
 X_t = X[1,],
 Mean_t_prev = colMeans(X[-1,]),
            = n - 1
colMeans(X)
# These two should be equal
cov_recursive(
 X_t = X[1, ],
Cov_t = cov(X[-1,]),
Mean_t = colMeans(X),
 Mean_t_prev = colMeans(X[-1, ]),
             = n-1
)
cov(X)
set.seed(13155511)
X \leftarrow matrix(rnorm(1e3*100), ncol = 100)
ans0 <- cov(X[-1,])
t0 <- system.time({</pre>
 ans1 <- cov(X)
})
t1 <- system.time(ans2 <- cov_recursive(</pre>
 X[1, ], ans0,
 Mean_t = colMeans(X),
 Mean_t_prev = colMeans(X[-1,]),
 t. = 1e3 - 1
))
# Comparing accuracy and speed
range(ans1 - ans2)
t0/t1
```

fmcmc 9

fmcmc

A friendly MCMC framework

Description

The fmcmc package provides a flexible framework for implementing MCMC models using a lightweight in terms of dependencies. Among its main features, fmcmc allows:

Details

- Implementing arbitrary transition kernels.
- Incorporating convergence monitors for automatic stop.
- Out-of-the-box parallel computing implementation for running multiple chains simultaneously.

For more information see the packages vignettes:

```
vignette("workflow-with-fmcmc", "fmcmc")
vignette("user-defined-kernels", "fmcmc")
```

References

Vega Yon et al., (2019). fmcmc: A friendly MCMC framework. Journal of Open Source Software, 4(39), 1427, doi:10.21105/joss.01427

fmcmc-deprecated

Deprecated methods in fmcmc

Description

These functions will no longer be included starting version 0.6-0. Instead, use the functions in mcmc-output.

Usage

```
last_elapsed()
LAST_MCMC
last_nsteps()
last_nchains()
```

10 kernel_adapt

```
last_kernel()
last_conv_checker()
last_(x)
```

Arguments

Х

Name of the object to retrieve.

Format

An object of class fmcmc_last_mcmc of length 0.

Value

The function last_elapsed returns the elapsed time of the last call to MCMC. In particular, the MCMC function records the running time of R at the beginning and end of the function using proc.time(). So this function returns the difference between the two (time_end - time_start).

kernel_adapt

Adaptive Metropolis (AM) Transition Kernel

Description

Implementation of Haario et al. (2001)'s Adaptive Metropolis.

Usage

```
kernel_adapt(
 mu = 0,
 bw = 0L.
 lb = -.Machine$double.xmax,
  ub = .Machine$double.xmax,
  freq = 1L,
 warmup = 500L
  Sigma = NULL,
  Sd = NULL,
  eps = 1e-04,
  fixed = FALSE,
  until = Inf
)
kernel_am(
 mu = 0,
 bw = 0L,
  lb = -.Machine$double.xmax,
  ub = .Machine$double.xmax,
```

kernel_adapt 11

```
freq = 1L,
warmup = 500L,
Sigma = NULL,
Sd = NULL,
eps = 1e-04,
fixed = FALSE,
until = Inf
)
```

Arguments

mu	Either a numeric vector or a scalar. Proposal mean. If scalar, values are recycled to match the number of parameters in the objective function.
bw	Integer scalar. The bandwidth, is the number of observations to include in the computation of the variance-covariance matrix.
lb, ub	Either a numeric vector or a scalar. Lower and upper bounds for bounded kernels. When of length 1, the values are recycled to match the number of parameters in the objective function.
freq	Integer scalar. Frequency of updates. How often the variance-covariance matrix is updated. The implementation is different from that described in the original paper (see details).
warmup	Integer scalar. The number of iterations that the algorithm has to wait before starting to do the updates.
Sigma	The variance-covariance matrix. By default this will be an identity matrix during the warmup period.
Sd	Overall scale for the algorithm. By default, the variance-covariance is scaled to $2.4^2/d$, with d the number of dimensions.
eps	Double scalar. Default size of the initial step (see details).
fixed	Logical scalar or vector of length k. Indicates which parameters will be treated as fixed or not. Single values are recycled.
until	Integer scalar. Last step at which adaptation takes place (see details).

Details

While it has been shown that under regular conditions this transition kernel generates ergodic chains even when the adaptation does not stop, some practitioners may want to stop adaptation at some point.

kernel_adapt Implements the adaptive Metropolis (AM) algorithm of Haario et al. (2001). If the value of bw is greater than zero, then the algorithm folds back AP, a previous version which is known to have ergodicity problems.

The parameter eps has two functions. The first one is to set the initial scale for the multivariate normal kernel, which is replaced after warmup steps with the actual variance-covariance computed by the main algorithm. The second usage is in the equation that ensures that the variance-covariance is greater than zero, this is, the ε parameter in the original paper.

The update of the covariance matrix is done using cov_recursive() function, which makes the updates faster. The freq parameter, besides of indicating the frequency with which the updates

12 kernel_mirror

are done, it specifies what are the samples included in each update, in other words, like a thinning parameter, only every freq samples will be used to compute the covariance matrix. Since this implementation uses the recursive formula for updating the covariance, there is no practical need to set freq != 1.

kernel_am is just an alias for kernel_adapt.

Value

An object of class fmcmc_kernel. fmcmc_kernel objects are intended to be used with the MCMC() function.

References

```
Haario, H., Saksman, E., & Tamminen, J. (2001). An adaptive Metropolis algorithm. Bernoulli, 7(2), 223–242. https://projecteuclid.org/euclid.bj/1080222083
```

See Also

```
Other kernels: kernel_mirror, kernel_new(), kernel_normal(), kernel_ram(), kernel_unif()
```

Examples

```
# Update every-step and wait 1,000 steps before starting to adapt
kern <- kernel_adapt(freq = 1, warmup = 1000)

# Two parameters model, the second parameter with a restricted range, i.e.
# a lower bound of 1
kern <- kernel_adapt(lb = c(-.Machine$double.xmax, 0))</pre>
```

kernel_mirror

Mirror Transition Kernels

Description

NMirror and UMirror transition kernels described in Thawornwattana et al. (2018).

Usage

```
kernel_nmirror(
  mu = 0,
  scale = 1,
  warmup = 500L,
  nadapt = 4L,
  arate = 0.4,
  lb = -.Machine$double.xmax,
  ub = .Machine$double.xmax,
  fixed = FALSE,
  scheme = "joint"
```

kernel_mirror 13

```
kernel_umirror(
   mu = 0,
   scale = 1,
   warmup = 500L,
   nadapt = 4L,
   arate = 0.4,
   lb = -.Machine$double.xmax,
   ub = .Machine$double.xmax,
   fixed = FALSE,
   scheme = "joint"
)
```

Arguments

mu, scale	Either a numeric vector or a scalar. Proposal mean and scale. If scalar, values are recycled to match the number of parameters in the objective function.
warmup	Integer. Number of steps required before starting adapting the chains.
nadapt	Integer. Number of times the scale is adjusted for adaptation during the warmup (burn-in) period.
arate	Double. Target acceptance rate used as a reference during the adaptation process.
1b, ub	Either a numeric vector or a scalar. Lower and upper bounds for bounded kernels. When of length 1, the values are recycled to match the number of parameters in the objective function.
fixed, scheme	For multivariate functions, sets the update plan. See plan_update_sequence().

Details

The kernel_nmirror and kernel_umirror functions implement simple symmetric transition kernels that pivot around an approximation of the asymptotic mean.

In the multidimensional case, this implementation just draws a vector of independent draws from the proposal kernel, instead of using, for example, a multivariate distribution of some kind. This will be implemented in the next update of the package.

During the warmup period (or burnin as described in the paper), the algorithm adapts both the scale and the reference mean of the proposal distribution. While the mean is adapted continuously, the scale is updated only a handful of times, in particular, nadapt times during the warmup time. The adaptation is done as proposed by Yang and Rodriguez (2013) in which the scale is adapted four times.

Value

An object of class fmcmc_kernel. fmcmc_kernel objects are intended to be used with the MCMC() function.

14 kernel_new

References

Thawornwattana, Y., Dalquen, D., & Yang, Z. (2018). Designing Simple and Efficient Markov Chain Monte Carlo Proposal Kernels. Bayesian Analysis, 13(4), 1037–1063. doi:10.1214/17-BA1084

Yang, Z., & Rodriguez, C. E. (2013). Searching for efficient Markov chain Monte Carlo proposal kernels. Proceedings of the National Academy of Sciences, 110(48), 19307–19312. doi:10.1073/pnas.1311790110

See Also

```
Other kernels: kernel_adapt(), kernel_new(), kernel_normal(), kernel_ram(), kernel_unif()
```

Examples

```
# Normal mirror kernel with 5 adaptations and 1000 steps of warmup (burnin)
kern <- kernel_nmirror(nadapt = 5, warmup = 1000)

# Same as before but using a uniform mirror and choosing a target acceptance
# rate of 24 %
kern <- kernel_umirror(nadapt = 5, warmup = 1000, arate = .24)</pre>
```

kernel_new

Transition Kernels for MCMC

Description

The function kernel_new is a helper function that allows creating fmcmc_kernel objects which are passed to the MCMC() function.

Usage

```
kernel_new(proposal, ..., logratio = NULL, kernel_env = new.env(hash = TRUE))
```

Arguments

```
proposal, logratio
```

Functions. Both receive a single argument, an environment. This functions are called later within MCMC (see details).

... In the case of kernel_new, further arguments to be stored with the kernel.

kernel_env

Environment. This will be used as the main container of the kernel's components. It is returned as an object of class c("environment", "fmcmc_kernel").

kernel_new 15

Details

The objects fmcmc_kernels are environments that in general contain the following objects:

• proposal: The function used to propose changes in the chain based on the current state. The function must return a vector of length equal to the number of parameters in the model.

• logratio: This function is called after a new state has been proposed, and is used to compute the log of the Hastings ratio.

In the case that the logratio function is not specified, then it is assumed that the transition kernel is symmetric, this is, log-ratio is then implemented as function(env) {env\$f1 - env\$f0}

• ...: Further objects that are used within those functions.

Both functions, proposal and logratio, receive a single argument, an environment, which is passed by the MCMC() function during each step using the function environment().

The passed environment is actually the environment in which the MCMC function is running, in particular, this environment contains the following objects:

Object Description i Integer. The current iteration. Numeric vector. The last proposed state. theta1 Numeric vector. The current state theta0 The log-unnormalized posterior function (a wrapper of fun passed to MCMC). f1 The last value of f(theta1) f0 The last value of f(theta0) The actual fmcmc_kernel object. kernel The matrix of samples defined up to i - 1. ans

These are the core component of the MCMC function. The following block of code is how this is actually implemented in the package:

```
for (i in 1L:nsteps) {
  # Step 1. Propose
  theta1[] <- kernel$proposal(environment())</pre>
           <- f(theta1)
  # Checking f(theta1) (it must be a number, can be Inf)
  if (is.nan(f1) | is.na(f1) | is.null(f1))
   stop(
      "fun(par) is undefined (", f1, ")",
      "Check either -fun- or the -lb- and -ub- parameters.",
      call. = FALSE
    )
 # Step 2. Hastings ratio
  if (R[i] < kernel$logratio(environment())) {</pre>
   theta0 <- theta1
    f0
           <- f1
```

16 kernel_new

```
}
# Step 3. Saving the state
ans[i,] <- theta0
}</pre>
```

For an extensive example on how to create new kernel objects see the vignette vignette ("user-defined-kernels", "fmcmc").

Value

An environment of class fmcmc_kernel which contains the following:

- proposal A function that receives a single argument, an environment. This is the proposal function used within MCMC().
- logratio A function to compute log ratios of the current vs the proposed step of the chain. Also used within MCMC().
- ... Further arguments passed to kernel_new.

Behavior

In some cases, calls to the proposal() and logratio() functions in fmcmc_kernels can trigger changes or updates of variables stored within them. A concrete example is with adaptive kernels.

Adaptive Metropolis and Robust Adaptive Metropolis implemented in the functions kernel_adapt() and kernel_ram() both update a covariance matrix used during the proposal stage, and furthermore, have a warmup stage that sets the point at which both will start adapting. Because of this, both kernels have internal counters of the absolute step count which allows them activating, scaling, etc. the proposals correctly.

- 1. When running multiple chains, MCMC will create independent copies of a baseline passed fmcmc_kernel object. These are managed together in a fmcmc_kernel_list object.
- 2. Even if the chains are run in parallel, if a predefined kernel object is passed it will be updated to reflect the last state of the kernels before the MCMC call returns.

References

Brooks, S., Gelman, A., Jones, G. L., & Meng, X. L. (2011). Handbook of Markov Chain Monte Carlo. Handbook of Markov Chain Monte Carlo.

See Also

Other kernels: kernel_adapt(), kernel_mirror, kernel_normal(), kernel_ram(), kernel_unif()

kernel_normal 17

Examples

```
# Example creating a multivariate normal kernel using the mytnorm R package
# for a bivariate normal distribution
library(mvtnorm)
# Define your Sigma
sigma <- matrix(c(1, .2, .2, 1), ncol = 2)
# How does it looks like?
sigma
       [,1] [,2]
# [1,] 1.0 0.2
# [2,] 0.2 1.0
# Create the kernel
kernel_mvn <- kernel_new(</pre>
  proposal = function(env) {
  env$theta0 + as.vector(mvtnorm::rmvnorm(1, mean = 0, sigma = sigma.))
  },
  sigma. = sigma
# As you can see, in the previous call we passed sigma as it will be used by
# the proposal function
# The logaratio function was not necesary to be passed since this kernel is
# symmetric.
```

kernel_normal

Gaussian Transition Kernel

Description

Gaussian Transition Kernel

Usage

```
kernel_normal(mu = 0, scale = 1, fixed = FALSE, scheme = "joint")
kernel_normal_reflective(
    mu = 0,
    scale = 1,
    lb = -.Machine$double.xmax,
    ub = .Machine$double.xmax,
    fixed = FALSE,
    scheme = "joint"
)
```

18 kernel_ram

Arguments

mu, scale	Either a numeric vector or a scalar. Proposal mean and scale. If scalar, values are recycled to match the number of parameters in the objective function.
fixed, scheme	For multivariate functions, sets the update plan. See plan_update_sequence().
1b, ub	Either a numeric vector or a scalar. Lower and upper bounds for bounded kernels. When of length 1, the values are recycled to match the number of parameters in the objective function.

Details

The kernel_normal function provides the canonical normal kernel with symmetric transition probabilities.

The kernel_normal_reflective implements the normal kernel with reflective boundaries. Lower and upper bounds are treated using reflecting boundaries, this is, if the proposed θ' is greater than the ub, then $\theta' - ub$ is subtracted from ub. At the same time, if it is less than 1b, then $lb - \theta'$ is added to 1b iterating until θ is within [1b, ub].

In this case, the transition probability is symmetric (just like the normal kernel).

Value

An object of class fmcmc_kernel. fmcmc_kernel objects are intended to be used with the MCMC() function.

See Also

```
Other kernels: kernel_adapt(), kernel_mirror, kernel_new(), kernel_ram(), kernel_unif()
```

Examples

```
# Normal kernel with a small scale (sd) of 0.05
kern <- kernel_normal(scale = 0.05)

# Using boundaries for the second parameter of a two parameter chain
# to have values in [0, 100].
kern <- kernel_normal_reflective(
   ub = c(.Machine$double.xmax, 100),
   lb = c(-.Machine$double.xmax, 0)
   )</pre>
```

kernel_ram

Robust Adaptive Metropolis (RAM) Transition Kernel

Description

Implementation of Vihola (2012)'s Robust Adaptive Metropolis.

kernel_ram 19

Usage

```
kernel_ram(
    mu = 0,
    eta = function(i, k) min(c(1, i^(-2/3) * k)),
    qfun = function(k) stats::rt(k, k),
    arate = 0.234,
    freq = 1L,
    warmup = 0L,
    Sigma = NULL,
    eps = 1e-04,
    lb = -.Machine$double.xmax,
    ub = .Machine$double.xmax,
    fixed = FALSE,
    until = Inf,
    constr = NULL
)
```

Arguments

mu	Either a numeric vector or a scalar. Proposal mean. If scalar, values are recycled to match the number of parameters in the objective function.
eta	A function that receives the MCMC environment. This is to calculate the scaling factor for the adaptation.
qfun	Function. As described in Vihola (2012)'s, the qfun function is a symmetric function used to generate random numbers.
arate	Numeric scalar. Objective acceptance rate.
freq	Integer scalar. Frequency of updates. How often the variance-covariance matrix is updated.
warmup	Integer scalar. The number of iterations that the algorithm has to wait before starting to do the updates.
Sigma	The variance-covariance matrix. By default this will be an identity matrix during the warmup period.
eps	Double scalar. Default size of the initial step (see details).
lb, ub	Either a numeric vector or a scalar. Lower and upper bounds for bounded kernels. When of length 1, the values are recycled to match the number of parameters in the objective function.
fixed	Logical scalar or vector of length k. Indicates which parameters will be treated as fixed or not. Single values are recycled.
until	Integer scalar. Last step at which adaptation takes place (see details).
constr	Logical lower-diagonal square matrix of size k. Not in the original paper, but rather a tweak that imposes a constraint on the S_n matrix. If different from NULL, the kernel multiplates S_n by this constraint so that zero elements are pre-imposed.

20 kernel_unif

Details

While it has been shown that under regular conditions this transition kernel generates ergodic chains even when the adaptation does not stop, some practitioners may want to stop adaptation at some point.

The idea is similar to that of the Adaptive Metropolis algorithm (AM implemented as kernel_adapt() here) with the difference that it takes into account a target acceptance rate.

The eta function regulates the rate of adaptation. The default implementation will decrease the rate of adaptation exponentially as a function of the iteration number.

$$Y_n \equiv X_{n-1} + S_{n-1} U_n, \quad {
m where} \ U_n \sim q \ {
m (the \ qfun)}$$

And the S_n matrix is updated according to the following equation:

$$S_n S_n^T = S_{n-1} \left(I + \eta_n (\alpha_n - \alpha_*) \frac{U_n U_n^T}{\|U_n\|^2} \right) S_{n-1}^T$$

Value

An object of class fmcmc_kernel.

References

Vihola, M. (2012). Robust adaptive Metropolis algorithm with coerced acceptance rate. Statistics and Computing, 22(5), 997–1008. doi:10.1007/s1122201192695

See Also

```
Other kernels: kernel_adapt(), kernel_mirror, kernel_new(), kernel_normal(), kernel_unif()
```

Examples

```
# Setting the acceptance rate to 30 % and deferring the updates until
# after 1000 steps
kern <- kernel_ram(arate = .3, warmup = 1000)</pre>
```

kernel_unif

Uniform Transition Kernel

Description

Uniform Transition Kernel

kernel_unif 21

Usage

```
kernel_unif(min. = -1, max. = 1, fixed = FALSE, scheme = "joint")
kernel_unif_reflective(
    min. = -1,
    max. = 1,
    lb = min.,
    ub = max.,
    fixed = FALSE,
    scheme = "joint"
)
```

Arguments

min., max. Passed to runif.

fixed, scheme For multivariate functions, sets the update plan. See plan_update_sequence().

lb, ub Either a numeric vector or a scalar. Lower and upper bounds for bounded kernels. When of length 1, the values are recycled to match the number of parameters in the objective function.

Details

The kernel_unif function provides a uniform transition kernel. This (symmetric) kernel function by default adds the current status values between [-1,1].

The kernel_unif_reflective is similar to kernel_unif with the main difference that proposals are bounded to be within [lb, ub].

Value

An object of class fmcmc_kernel. fmcmc_kernel objects are intended to be used with the MCMC() function.

See Also

```
Other kernels: kernel_adapt(), kernel_mirror, kernel_new(), kernel_normal(), kernel_ram()
```

Examples

```
# Multivariate setting with 4 parameters in which we set the kernel to make
# proposals one parameter at-a-time in a random ordering.
kern <- kernel_unif(scheme = "random")</pre>
```

22 lifeexpect

lifeexpect

Life expectancy in the US (2020)

Description

A simulated data set based on statistics of life expectancy in the US at birth.

Usage

lifeexpect

Format

A 1.000 rows data frame with three columns:

- · age: Years lived.
- smoke: 0/1 variable equal to 1 if the individual smokes.
- female: 0/1 variable equal to 1 if the individual is a female at birth.

Details

The data was generated using official statistics from the CDC and a study of life expectancy of smokers in the US published in the New England Journal of Medicine (see references).

According to the CDC, data from 2020 indicates that the average life expectancy of females in the US is 80.5 years vs 75.1 years for males (which declined with respect to 2019 after COVID hit the US). In Jha et al. (2013), evidence is presented indicating that individuals who smoke have at least ten years left of life expectancy compared to non-smokers.

The parameter estimates for the data generating process where:

- An average of life expectancy of 80.1.
- Smokers live 10 years less than non-smokers.
- Females live 5.4 years longer than males.

References

Jha, P., Ramasundarahettige, C., Landsman, V., Rostron, B., Thun, M., Anderson, R. N., ... Peto, R. (2013). 21st-Century Hazards of Smoking and Benefits of Cessation in the United States. New England Journal of Medicine, 368(4), 341–350. doi:10.1056/NEJMsa1211128

Arias, E., Tejada-Vera, B., & Ahmad, F. (2021). Provisional life expectancy estimates for January through June, 2020. https://www.cdc.gov/nchs/data/vsrr/VSRR10-508.pdf

MCMC

Markov Chain Monte Carlo

Description

A flexible implementation of the Metropolis-Hastings MCMC algorithm, users can utilize arbitrary transition kernels as well as set-up an automatic stop criterion using a convergence check test.

Usage

```
MCMC(
  initial,
  fun,
  nsteps,
  . . . ,
  seed = NULL,
  nchains = 1L,
  burnin = 0L,
  thin = 1L,
  kernel = kernel_normal(),
  multicore = FALSE,
  conv_checker = NULL,
  cl = NULL,
  progress = interactive() && !multicore,
  chain_id = 1L
MCMC_without_conv_checker(
  initial,
  fun,
  nsteps,
  nchains = 1L,
  burnin = 0L,
  thin = 1L,
  kernel = kernel_normal(),
  multicore = FALSE,
  conv_checker = NULL,
  cl = NULL,
  progress = interactive() && !multicore,
  chain_id = 1L
)
MCMC_OUTPUT
```

Arguments

initial Either a numeric matrix or vector, or an object of class coda::mcmc or coda::mcmc.list

(see details). initial values of the parameters for each chain (See details).

fun A function. Returns the log-likelihood.

nsteps Integer scalar. Length of each chain.

... Further arguments passed to fun.

seed If not null, passed to set.seed.

nchains Integer scalar. Number of chains to run (in parallel).

burnin Integer scalar. Length of burn-in. Passed to coda::mcmc as start.

thin Integer scalar. Passed to coda::mcmc. kernel An object of class fmcmc_kernel.

multicore Logical. If FALSE then chains will be executed in serial.

conv_checker A function that receives an object of class coda::mcmc.list, and returns a logical

value with TRUE indicating convergence. See the "Automatic stop" section and

the convergence-checker manual.

cl A cluster object passed to parallel::clusterApply.

progress Logical scalar. When set to TRUE shows a progress bar. A new bar will be show

every time that the convergence checker is called.

chain_id Integer scalar (internal use only). This is an argument passed to the kernel func-

tion and it allows it identify in which of the chains the process is taking place.

This could be relevant for some kernels (see kernel_new()).

Details

This function implements Markov Chain Monte Carlo (MCMC) using the Metropolis-Hastings ratio with flexible transition kernels. Users can specify either one of the available transition kernels or define one of their own (see kernels). Furthermore, it allows easy parallel implementation running multiple chains in parallel. The function also allows using convergence diagnostics tests to set-up a criterion for automatically stopping the algorithm (see convergence-checker).

The canonical form of the Metropolis Hastings algorithm consists on accepting a move from state x to state y based on the Hastings ratio r(x,y):

$$r(x,y) = \frac{h(y)q(y,x)}{h(x)q(x,y)},$$

where h is the unnormalized density of the specified distribution (the posterior probability), and q has the conditional probability of moving from state x to y (the proposal density). The move $x \to y$ is then accepted with probability

$$\alpha(x, y) = \min(1, r(x, y))$$

Observe that, in the case that q() is symmetric, meaning q(x,y)=q(y,x), the Hastings ration reduces to h(y)/h(x). Starting version 0.5-0, the value of the log unnormalized density and the proposed states y can be accessed using the functions get_logpost() and get_draws().

We now give details of the various options included in the function.

The function MCMC_without_conv_checker is for internal use only.

Value

MCMC returns an object of class coda::mcmc from the **coda** package. The mcmc object is a matrix with one column per parameter, and nsteps rows. If nchains > 1, then it returns a coda::mcmc.list.

While the main output of MCMC is the mcmc(.list) object, other information and intermediate outputs of the process are stored in MCMC_OUTPUT. For information about how to retrieve/set data, see mcmc-output.

Starting point

By default, if initial is of class mcmc, MCMC will take the last nchains points from the chain as starting point for the new sequence. If initial is of class mcmc.list, the number of chains in initial must match the nchains parameter.

If initial is a vector, then it must be of length equal to the number of parameters used in the model. When using multiple chains, if initial is not an object of class mcmc or mcmc.list, then it must be a numeric matrix with as many rows as chains, and as many columns as parameters in the model.

Multiple chains

When nchains > 1, the function will run multiple chains. Furthermore, if cl is not passed, MCMC will create a PSOCK cluster using makePSOCKcluster with parallel::detectCores clusters and attempt to execute using multiple cores. Internally, the function does the following:

When running in parallel, objects that are used within fun must be passed through ..., otherwise the cluster will return with an error.

The user controls the initial value of the parameters of the MCMC algorithm using the argument initial. When using multiple chains, i.e., nchains > 1, the user can specify multiple starting points, which is recommended. In such a case, each row of initial is use as a starting point for each of the chains. If initial is a vector and nchains > 1, the value is recycled, so all chains start from the same point (not recommended, the function throws a warning message).

Automatic stop

By default, no automatic stop is implemented. If one of the functions in convergence-checker is used, then the MCMC is done by bulks as specified by the convergence checker function, and thus the algorithm will stop if, the conv_checker returns TRUE. For more information see convergence-checker.

References

Brooks, S., Gelman, A., Jones, G. L., & Meng, X. L. (2011). Handbook of Markov Chain Monte Carlo. Handbook of Markov Chain Monte Carlo.

Vega Yon, G., & Marjoram, P. (2019). fmcmc: A friendly MCMC framework. Journal of Open Source Software, 4(39), 1427. doi:10.21105/joss.01427

See Also

get_logpost(), get_logpost() (mcmc-output) for post execution of MCMC, and ith_step() for accessing objects within an MCMC call.

Examples

```
# Univariate distributed data with multiple parameters ------
# Parameters
set.seed(1231)
n <- 1e3
pars <- c(mean = 2.6, sd = 3)
# Generating data and writing the log likelihood function
D <- rnorm(n, pars[1], pars[2])</pre>
fun <- function(x) {</pre>
  x \leftarrow log(dnorm(D, x[1], x[2]))
  sum(x)
}
# Calling MCMC, but first, loading the coda R package for
# diagnostics
library(coda)
ans <- MCMC(
  fun, initial = c(mu=1, sigma=1), nsteps = 2e3,
  kernel = kernel_normal_reflective(scale = .1, ub = 10, lb = 0)
# Ploting the output
oldpar <- par(no.readonly = TRUE)</pre>
par(mfrow = c(1,2))
boxplot(as.matrix(ans),
        main = expression("Posterior distribution of"~mu~and~sigma),
        names = expression(mu, sigma), horizontal = TRUE,
        col = blues9[c(4,9)],
        sub = bquote(mu == .(pars[1])~", and"~sigma == .(pars[2]))
abline(v = pars, col = blues9[c(4,9)], lwd = 2, lty = 2)
plot(apply(as.matrix(ans), 1, fun), type = "1",
     main = "LogLikelihood",
    ylab = expression(L("{"~mu,sigma~"}"~"|"~D))
)
par(oldpar)
```

```
# In this example we estimate the parameter for a dataset with ---------
# With 5,000 draws from a MVN() with parameters M and S.
# Loading the required packages
library(mvtnorm)
library(coda)
# Parameters and data simulation
S \leftarrow cbind(c(.8, .2), c(.2, 1))
M < -c(0, 1)
set.seed(123)
D <- rmvnorm(5e3, mean = M, sigma = S)
# Function to pass to MCMC
fun <- function(pars) {</pre>
 # Putting the parameters in a sensible way
 m <- pars[1:2]</pre>
 s <- cbind( c(pars[3], pars[4]), c(pars[4], pars[5]) )</pre>
 # Computing the unnormalized log likelihood
 sum(log(dmvnorm(D, m, s)))
}
# Calling MCMC
ans <- MCMC(
 initial = c(mu0=5, mu1=5, s0=5, s01=0, s2=5),
 kernel = kernel_normal_reflective(
   1b = c(-10, -10, .01, -5, .01),
   ub = 5,
   scale = 0.01
 ),
 nsteps = 1e3,
 thin = 10,
 burnin = 5e2
)
# Checking out the outcomes
plot(ans)
summary(ans)
# Multiple chains -----------
# As we want to run -fun- in multiple cores, we have to
# pass -D- explicitly (unless using Fork Clusters)
# just like specifying that we are calling a function from the
# -mvtnorm- package.
fun <- function(pars, D) {</pre>
 # Putting the parameters in a sensible way
 m <- pars[1:2]</pre>
```

```
s <- cbind( c(pars[3], pars[4]), c(pars[4], pars[5]) )</pre>
 # Computing the unnormalized log likelihood
 sum(log(mvtnorm::dmvnorm(D, m, s)))
}
# Two chains
ans <- MCMC(
 initial = c(mu0=5, mu1=5, s0=5, s01=0, s2=5),
 nchains = 2,
 kernel = kernel_normal_reflective(
         = c(-10, -10, .01, -5, .01),
   ub
        = 5,
   scale = 0.01
 ),
 nsteps = 1e3,
 thin
         = 10,
 burnin = 5e2,
 D
         = D
)
summary(ans)
```

mcmc-loop

Functions to interact with the main loop

Description

You can use these functions to read variables, store, and retrieve data during the MCMC process.

Usage

```
ith_step(x)
set_userdata(...)
get_userdata()
```

Arguments

x Name of the element to retrieve. If missing, it will return the entire environment in which the main MCMC loop is running.

... Named values to be appended to the user data.

Value

The function ith_step() provides access to the following elements:

- i : (int) Step (iteration) number.
- nsteps: (int) Number of steps.
- chain_id: (int) Id of the chain (goes from 1 to -nchains-)
- theta0: (double vector) Current state of the chain.
- theta1 : (double vector) Proposed state of the chain.
- ans : (double matrix) Set of accepted states (it will be NA for rows >= i).
- draws : (double matrix) Set of proposed states (it will be NA for rows >= i).
- logpost : (double vector) Value of -fun- (it will be NA for elements >= i).
- R: (double vector) Random values from U(0,1). This is used with the Hastings ratio.
- thin: (int) Thinning (applied after the last step).
- burnin: (int) Burn-in (applied after the last step).
- conv_checker : (function) Convergence checker function.
- kernel : (fmcmc_kernel) Kernel object.
- fun: (function) Passed function to MCMC.
- f: (function) Wrapper of -fun-.
- initial: (double vector) Starting point of the chain.

The following objects always have fixed values (see ?ith_step): nchains, cl, multicore

Other available objects: cnames, funargs, MCMC_OUTPUT, passedargs, progress

The function set_userdata() returns invisible(). The only side effect is appending the information by row.

Advanced usage

The function ith_step() is a convenience function that provides access to the environment within which the main loop of the MCMC call is being evaluated. This is a wrapper of MCMC_OUTPUT\$loop_envir that will either return the value x or, if missing, the entire environment. If ith_step() is called outside of the MCMC call, then it will return with an error.

For example, if you wanted to print information if the current value of logpost is greater than the previous value of logpost, you could define the objective function as follows:

```
return(logpost_curr)
}
```

In the case of the objects nchains, cl, and multicore, the function will always return the default values 1, NULL, and FALSE, respectively. Thus, the user shouldn't rely on these objects to provide information regarding runs using multiple chains. More examples below.

Examples

```
#' # Getting the logpost -------
set.seed(23133)
x <- rnorm(200)
y < -x*2 + rnorm(200)
f <- function(p) {</pre>
 sum(dnorm(y - x*p, log = TRUE))
}
ans <- MCMC(fun = f, initial = c(0), nsteps=2000)
plot(get_logpost(), type = "1") # Plotting the logpost from the last run
# Printing information every 500 step ------
# for this we use ith_step()
f <- function(p) {
 # Capturing info from within the loop
      <- ith_step("i")
 nsteps <- ith_step("nsteps")</pre>
 if (!(i %% 500)) {
    "Step ", i, " of ", nsteps,". Values in the loop:\n",
    "theta0: ", ith_step("theta0"), "\n",
    "theta1: ", ith_step()theta1, "\n",
    sep = ""
   )
 }
 sum(dnorm(y - x*p, log = TRUE))
}
ans0 <- MCMC(fun = f, initial = c(0), nsteps=2000, progress = FALSE, seed = 22)
# Step 500 of 2000. Values in the loop:
# theta0: 2.025379
# theta1: 1.04524
```

```
# Step 1000 of 2000. Values in the loop:
# theta0: 2.145967
# theta1: 0.2054037
# Step 1500 of 2000. Values in the loop:
# theta0: 2.211691
# theta1: 2.515361
# Step 2000 of 2000. Values in the loop:
# theta0: 1.998789
# theta1: 1.33034
# Printing information if the current logpost is greater than max -------
f <- function(p) {</pre>
             <- ith_step("i")
 logpost_prev <- max(ith_step("logpost")[1:(i-1)])</pre>
 logpost_curr <- sum(dnorm(y - x*p, log = TRUE))</pre>
 # Only worthwhile after the first step
 if ((i > 1L) && logpost_prev < logpost_curr)</pre>
   cat("At a higher point!:", logpost_curr, ", step:", i,"\n")
 return(logpost_curr)
ans1 <- MCMC(fun = f, initial = c(0), nsteps=1000, progress = FALSE, seed = 22)
# At a higher point!: -357.3584 , step: 2
# At a higher point!: -272.6816 , step: 6
# At a higher point!: -270.9969 , step: 7
# At a higher point!: -269.8128 , step: 24
# At a higher point!: -269.7435 , step: 46
# At a higher point!: -269.7422 , step: 543
# At a higher point!: -269.7421 , step: 788
# Saving extra information ------
data("lifeexpect")
# Defining the logposterior
logpost <- function(p) {</pre>
 # Reconding the sum of the parameters (just because)
 # and the number of step.
 set_userdata(i = ith_step("i"), sum_of_p = sum(p))
 with(lifeexpect, {
   sum(dnorm(age - (p[1] + p[2]*smoke + p[3]*female), sd = p[4], log = TRUE))
 })
}
# A kernel where sd is positive, the first is average age, so we
# make it positive too
```

32 mcmc-output

```
kern <- kernel_ram(lb = c(10, -20, -20, .0001), eps = .01)
ans <- MCMC(
   initial = c(70, -2, 2, 1), fun = logpost, kernel = kern, nsteps = 1000, seed = 1
   )

# Retrieving the data
head(get_userdata())

# It also works using multiple chains
ans_two <- MCMC(
   initial = c(70, -2, 2, 1), fun = logpost, kernel = kern, nsteps = 1000, seed = 1, nchains = 2
   )

user_dat <- get_userdata()
lapply(user_dat, head)</pre>
```

mcmc-output

Information about the last MCMC call

Description

This environment holds a copy of the last call to MCMC, including the start and end time (to compute total elapsed time) of the call. Since the resulting object of MCMC is an object of class coda::mcmc, this is a way to capture more information in case the user needs it.

Usage

```
get_(x)
get_logpost()
get_draws()
get_elapsed()
get_initial()
get_fun()
get_nsteps()
get_seed()
get_nchains()
get_burnin()
```

mcmc-output 33

```
get_thin()
get_kernel()
get_multicore()
get_conv_checker()
get_cl()
get_progress()
get_chain_id()
```

Arguments

Χ

Character scalar. Name of an argument to retrieve. If x was not passed to the last call, the function returns with an error.

Details

The function get_logpost returns the logposterior value at each iteration. The values correspond to a named numeric vector. If nchains > 1 then it will return a list of length nchains with the corresponding logpost values for each chain.

The function get_draws() retrieves the proposed states from the kernel function.

Examples

```
# Getting the logpost ------
set.seed(23133)
x <- rnorm(200)
y < -4 + x*2 + rnorm(200)
f <- function(p) {</pre>
 sum(dnorm(y - p[1] - x*p[2], log = TRUE))
}
# Setting a RAM kernel
kern <- kernel_am(eps = 1e-2)</pre>
ans <- MCMC(fun = f, initial = c(0, 1), nsteps = 2000, kernel = kern)
plot(
 # Plotting the logpost from the last run
 -get_logpost(),
 # Getting the number of chains
 main = paste0("nchains: ", get_nchains()),
 # And the elapsed time
 sub = sprintf("Run time: %.4f(s)", get_elapsed()[3]),
 type = "1",
 log = "y"
)
```

34 new_progress_bar

```
# This also works using multiple chains
ans <- MCMC(fun = f, initial = c(0, 0), nsteps=2000, nchains = 2, kernel = kern)
# In this case, just like -ans-,
draws <- get_draws()

# Plotting proposed points vs accepted
plot(
    draws[[1]], pch = 20,
    col = adjustcolor("gray", alpha = .5),
    main = "Accepted vs proposed states\n(chain 1)"
    )
lines(ans[[1]], pch = 20, col = "tomato", lwd = 2)
legend(
    "topleft", legend = c("Accepted", "Proposed"), pch = c(NA, 20),
    col = c("tomato", "black"), lty = c(1, NA), lwd = c(2, NA)
)</pre>
```

new_progress_bar

Progress bar

Description

A simple progress bar. This function is used in MCMC when the function has been called with a single processor.

Usage

```
new_progress_bar(
   n,
   probs = c(0, 0.25, 0.5, 0.75, 1),
   width = getOption("width", 80),
   symbol = "/",
   ...
)
```

Arguments

n	Integer. Number of steps.
probs	Double vector. Quantiles where to put marks
width	Integer. Width of the bar in characters.
symbol	Character. Single character symbol to print each bar.
	Further arguments passed to cat() such as file and append.

plan_update_sequence 35

Value

A function that can be included at the interior of a loop to mark the progress of the loop. It receives a single argument, i, which is the number of the current step.

Examples

```
x <- new_progress_bar(20)
for (i in 1:20) {
   Sys.sleep(2/20)
   x(i)
}</pre>
```

plan_update_sequence

Parameters' update sequence

Description

Parameters' update sequence

Usage

```
plan_update_sequence(k, nsteps, fixed, scheme)
```

Arguments

k Integer. Number of parameters nsteps Integer. Number of steps.

fixed Logical scalar or vector of length k. Indicates which parameters will be treated

as fixed or not. Single values are recycled.

scheme in which the proposals are made (see details).

Details

The parameter scheme present on the currently available kernels sets the way in which proposals are made. By default, scheme = "joint", proposals are done jointly, this is, at each step of the chain we are proposing new states for each parameter of the model. When scheme = "ordered", a sequential update schema is followed, in which, at each step of the chain, proposals are made one variable at a time, If scheme = "random", proposals are also made one variable at a time but in a random scheme.

Finally, users can specify their own sequence of proposals for the variables by passing a numeric vector to scheme, for example, if the user wants to make sequential proposals following the scheme 2, 1, 3, then scheme must be set to be scheme 2, 1, 3.

Value

A logical vector of size nsteps x k.

reflect_on_boundaries

Description

Adjust a proposal according to its support by reflecting it. This is the workhorse of kernel_normal_reflective and kernel_unif_reflective. It is intended for internal use only.

Usage

```
reflect_on_boundaries(x, lb, ub, which)
```

Arguments

x A numeric vector. The proposal

1b, ub Numeric vectors of length length(x). Lower and upper bounds.

which Integer vector. Index of variables to be updated.

Value

An adjusted proposal vector.

Index

* datasets	<pre>cov_recursive, 7</pre>	
convergence-checker, 4	<pre>cov_recursive(), 11</pre>	
fmcmc-deprecated, 9		
lifeexpect, 22	environment(), <i>15</i>	
MCMC, 23	6	
* kernels	fmcmc, 9	
kernel_adapt, 10	fmcmc-deprecated, 9	
kernel_mirror, 12	fmcmc-package (fmcmc), 9	
kernel_new, 14	fmcmc_kernel, 12, 13, 18, 20, 21, 24	
kernel_normal, 17	<pre>fmcmc_kernel (kernel_new), 14</pre>	
kernel_ram, 18	get(), 4	
kernel_unif, 20	get_ (mcmc-output), 32	
	get_burnin (mcmc-output), 32	
append_chains, 2	get_chain_id (mcmc-output), 32	
automatic-stop (convergence-checker), 4	get_cl (mcmc-output), 32	
	get_conv_checker (mcmc-output), 32	
cat(), 34	get_draws (mcmc-output), 32	
check_initial, 3	get_draws(), 24	
coda::gelman.diag(),5	get_elapsed (mcmc-output), 32	
coda::geweke.diag, 5	get_fun (mcmc-output), 32 get_initial (mcmc-output), 32 get_kernel (mcmc-output), 32 get_logpost (mcmc-output), 32	
coda::heidel.diag,5		
coda::mcmc, 2, 24, 25, 32		
coda::mcmc.list, 24, 25		
convergence-checker, 4, 24, 25	get_logpost(), 24, 26	
convergence_auto (convergence-checker),	<pre>get_multicore (mcmc-output), 32</pre>	
4	<pre>get_nchains (mcmc-output), 32</pre>	
convergence_data_get	<pre>get_nsteps (mcmc-output), 32</pre>	
(convergence-checker), 4	<pre>get_progress (mcmc-output), 32</pre>	
convergence_data_set	<pre>get_seed (mcmc-output), 32</pre>	
(convergence-checker), 4	<pre>get_thin (mcmc-output), 32</pre>	
convergence_gelman	<pre>get_userdata (mcmc-loop), 28</pre>	
(convergence-checker), 4		
convergence_geweke	invisible(), 29	
(convergence-checker), 4	ith_step(mcmc-loop), 28	
convergence_heildel	ith_step(), 26, 29	
(convergence-checker), 4	liannal adapt 10 14 16 19 20 21	
convergence_msg_get	kernel_adapt, 10, 14, 16, 18, 20, 21	
(convergence-checker), 4	kernel_adapt(), 7, 16, 20	
convergence_msg_set	kernel_am (kernel_adapt), 10	
(convergence-checker), 4	kernel_mirror, 12, 12, 16, 18, 20, 21	

38 INDEX

```
kernel_new, 12, 14, 14, 18, 20, 21
kernel_new(), 24
kernel_nmirror (kernel_mirror), 12
kernel_normal, 12, 14, 16, 17, 20, 21
kernel_normal_reflective, 36
kernel_normal_reflective
        (kernel_normal), 17
kernel_ram, 12, 14, 16, 18, 18, 21
kernel_ram(), 16
kernel_umirror (kernel_mirror), 12
kernel_unif, 12, 14, 16, 18, 20, 20
kernel_unif_reflective, 36
kernel_unif_reflective (kernel_unif), 20
kernels, 24
kernels (kernel_new), 14
last_(fmcmc-deprecated), 9
LAST_CONV_CHECK (convergence-checker), 4
last_conv_checker (fmcmc-deprecated), 9
last_elapsed (fmcmc-deprecated), 9
last_kernel (fmcmc-deprecated), 9
LAST_MCMC (fmcmc-deprecated), 9
last_nchains (fmcmc-deprecated), 9
last_nsteps (fmcmc-deprecated), 9
lifeexpect, 22
makePSOCKcluster, 25
MCMC, 4, 5, 10, 14, 15, 23, 32, 34
MCMC(), 12–16, 18, 21
mcmc-loop, 28
mcmc-output, 9, 25, 26, 32
MCMC_OUTPUT (MCMC), 23
MCMC_without_conv_checker (MCMC), 23
mean_recursive (cov_recursive), 7
Metropolis-Hastings (MCMC), 23
new_progress_bar, 34
parallel::clusterApply, 24
parallel::detectCores, 25
plan_update_sequence, 35
plan_update_sequence(), 13, 18, 21
proc.time(), 10
rbind, 2
reflect_on_boundaries, 36
runif, 21
set.seed, 24
set_userdata(mcmc-loop), 28
set_userdata(), 29
```