Package 'adaptMCMC'

January 30, 2024

Type Package

Title Implementation of a Generic Adaptive Monte Carlo Markov Chain Sampler

Version 1.5

Date 2024-01-29

Author Andreas Scheidegger, <andreas.scheidegger@eawag.ch>, <scheidegger.a@gmail.com>

Maintainer Andreas Scheidegger <andreas.scheidegger@eawag.ch>

Description Enables sampling from arbitrary distributions if the log density is known up to a constant; a common situation in the context of Bayesian inference. The implemented sampling algorithm was proposed by Vihola (2012) <DOI:10.1007/s11222-011-9269-5> and achieves often a high efficiency by tuning the proposal distributions to a user defined acceptance rate.

License GPL (>= 2)

LazyLoad yes

Depends R (>= 2.14.1), parallel, coda, Matrix

Imports ramcmc

URL https://github.com/scheidan/adaptMCMC

BugReports https://github.com/scheidan/adaptMCMC/issues

RoxygenNote 7.1.1

NeedsCompilation no

Repository CRAN

Date/Publication 2024-01-29 23:50:15 UTC

R topics documented:

adaptMCMC-package 2
convert.to.coda 2
MCMC 4
MCMC.add.samples 7
MCMC.parallel 8

Index **11**

adaptMCMC-package *Generic adaptive Monte Carlo Markov Chain sampler*

Description

Enables sampling from arbitrary distributions if the log density is known up to a constant; a common situation in the context of Bayesian inference. The implemented sampling algorithm was proposed by Vihola (2012) and achieves often a high efficiency by tuning the proposal distributions to a user defined acceptance rate.

Details

Package:	adaptMCMC
Type:	Package
Version:	1.4
Date:	2021-03-29
License:	GPL (>= 2)
LazyLoad:	yes

The workhorse function is `MCMC`. Chains can be updated with `MCMC.add.samples`. `MCMC.parallel` is a wrapper to generate independent chains on several CPU's in parallel using **parallel**. **coda**-functions can be used after conversion with `convert.to.coda`.

Author(s)

Andreas Scheidegger, <andreas.scheidegger@eawag.ch> or <scheidegger.a@gmail.com>

References

Vihola, M. (2012) Robust adaptive Metropolis algorithm with coerced acceptance rate. Statistics and Computing, 22(5), 997-1008. doi:10.1007/s11222-011-9269-5.

See Also

`MCMC`, `MCMC.add.samples`, `MCMC.parallel`, `convert.to.coda`

convert.to.coda *Converts chain(s) into* **coda** *objects.*

Description

Converts chain(s) produced by `MCMC` or `MCMC.parallel` into **coda** objects.

Usage

```
convert.to.coda(sample)
```

Arguments

sample	output of MCMC or MCMC.parallel.

Details

Converts chain(s) produced by MCMC or MCMC.parallel so that they can be used with functions of the **coda** package.

Value

An object of the class mcmc or mcmc.list.

Author(s)

Andreas Scheidegger, <andreas.scheidegger@eawag.ch> or <scheidegger.a@gmail.com>

See Also

MCMC, mcmc, mcmc.list

Examples

```
## ----------------------
## Banana shaped distribution

## log-pdf to sample from
p.log <- function(x) {
  B <- 0.03                               # controls 'bananacity'
  -x[1]^2/200 - 1/2*(x[2]+B*x[1]^2-100*B)^2
}


## ----------------------
## generate 200  samples

samp <- MCMC(p.log, n=200, init=c(0, 1), scale=c(1, 0.1),
               adapt=TRUE, acc.rate=0.234)


## ----------------------
## convert in object of class 'mcmc'
samp.coda <- convert.to.coda(samp)

class(samp.coda)

## ----------------------
## use functions of package 'coda'
```

```
require(coda)

plot(samp.coda)
cumuplot(samp.coda)
```

MCMC *(Adaptive) Metropolis Sampler*

Description

Implementation of the robust adaptive Metropolis sampler of Vihola (2012).

Usage

```
MCMC(p, n, init, scale = rep(1, length(init)),
    adapt = !is.null(acc.rate), acc.rate = NULL, gamma = 2/3,
    list = TRUE, showProgressBar=interactive(), n.start = 0, ...)
```

Arguments

p	function that returns a value proportional to the log probability density to sample from. Alternatively it can be a function that returns a list with at least one element named `log.density`. See details below.
n	number of samples.
init	vector with initial values.
scale	vector with the variances *or* covariance matrix of the jump distribution.
adapt	if `TRUE`, adaptive sampling is used, if `FALSE` classic metropolis sampling, if a positive integer the adaption stops after `adapt` iterations.
acc.rate	desired acceptance rate (ignored if `adapt=FALSE`)
gamma	controls the speed of adaption. Should be between 0.5 and 1. A lower gamma leads to faster adaption.
list	logical. If `TRUE` a list is returned otherwise only a matrix with the samples.
showProgressBar	logical. If `TRUE` a progress bar is shown.
n.start	iteration where the adaption starts. Only internally used.
...	further arguments passed to `p`.

Details

The algorithm tunes the covariance matrix of the (normal) jump distribution to achieve the desired acceptance rate. Classic (non-adaptive) Metropolis sampling can be obtained by setting `adapt=FALSE`.

Note, due to the calculation for the adaption steps the sampler is rather slow. However, with a suitable jump distribution good mixing can be observed with less samples. This is crucial if the computation of `p` is slow.

In some cases the function `p` may not only calculate the log density but return a list containing also other values. For example if `p` is a log posterior one may be also interested to store the corresponding prior and likelihood values. The function must either return always a scalar or always a list, however, the length of the list may vary.

Value

If `list=FALSE` a matrix is with the samples.

If `list=TRUE` a list is returned with the following components:

`samples`	matrix with samples
`log.p`	vector with the (unnormalized) log density for each sample
`n.sample`	number of generated samples
`acceptance.rate`	acceptance rate
`adaption`	either logical if adaption was used or not, or the number of adaption steps.
`sampling.parameters`	a list with further sampling parameters. Mainly used by `MCMC.add.samples()`
.	
`extra.values`	A list containing additional return values provided by `p`. Only if `p` provides a list.

Note

Due to numerical errors it may happen that the computed covariance matrix is not positive definite. In such a case the nearest positive definite matrix is calculated with `nearPD()` from the package **Matrix**.

Author(s)

Andreas Scheidegger, <andreas.scheidegger@eawag.ch> or <scheidegger.a@gmail.com>.

Thanks to David Pleydell, Venelin, and Umberto Picchini for spotting errors and providing improvements. Ian Taylor implemented the usage of `adapt_S` which lead to a nice speedup.

References

Vihola, M. (2012) Robust adaptive Metropolis algorithm with coerced acceptance rate. Statistics and Computing, 22(5), 997-1008. doi:10.1007/s11222-011-9269-5.

See Also

MCMC.parallel, MCMC.add.samples

Examples

```
## ----------------------
## Banana shaped distribution

## log-pdf to sample from
p.log <- function(x) {
  B <- 0.03                              # controls 'bananacity'
  -x[1]^2/200 - 1/2*(x[2]+B*x[1]^2-100*B)^2
}


## ----------------------
## generate samples

## 1) non-adaptive sampling
samp.1 <- MCMC(p.log, n=200, init=c(0, 1), scale=c(1, 0.1),
               adapt=FALSE)

## 2) adaptive sampling
samp.2 <- MCMC(p.log, n=200, init=c(0, 1), scale=c(1, 0.1),
               adapt=TRUE, acc.rate=0.234)


## ----------------------
## summarize results

str(samp.2)
summary(samp.2$samples)

## covariance of last jump distribution
samp.2$cov.jump


## ----------------------
## plot density and samples

x1 <- seq(-15, 15, length=80)
x2 <- seq(-15, 15, length=80)
d.banana <- matrix(apply(expand.grid(x1, x2), 1,  p.log), nrow=80)

par(mfrow=c(1,2))
image(x1, x2, exp(d.banana), col=cm.colors(60), asp=1, main="no adaption")
contour(x1, x2, exp(d.banana), add=TRUE, col=gray(0.6))
lines(samp.1$samples, type='b', pch=3)

image(x1, x2, exp(d.banana), col=cm.colors(60), asp=1, main="with adaption")
contour(x1, x2, exp(d.banana), add=TRUE, col=gray(0.6))
lines(samp.2$samples, type='b', pch=3)
```

```
## ----------------------
## function returning extra information in a list


p.log.list <- function(x) {
  B <- 0.03                             # controls 'bananacity'
  log.density <- -x[1]^2/200 - 1/2*(x[2]+B*x[1]^2-100*B)^2

  result <- list(log.density=log.density)

  ## under some conditions one may want to return other infos
  if(x[1]<0) {
    result$message <- "Attention x[1] is negative!"
    result$x <- x[1]
  }

  result
}

samp.list <- MCMC(p.log.list, n=200, init=c(0, 1), scale=c(1, 0.1),
                  adapt=TRUE, acc.rate=0.234)

## the additional values are stored under `extras.values`
head(samp.list$extras.values)
```

`MCMC.add.samples` *Add samples to an existing chain.*

Description

Add samples to an existing chain produced by `MCMC` or `MCMC.parallel`.

Usage

```
MCMC.add.samples(MCMC.object, n.update, ...)
```

Arguments

`MCMC.object`	a list produced by `MCMC` or `MCMC.parallel` with option `list = TRUE`.
`n.update`	number of additional samples.
`...`	further arguments passed to p.

Details

Only objects generated with the option `list = TRUE` can be updated.

A list of chains produced by `MCMC.parallel` can be updated. However, the calculations are *not* performed in parallel (i.e. only a single CPU is used).

Value

A updated version of `MCMC.object`.

Author(s)

Andreas Scheidegger, <andreas.scheidegger@eawag.ch> or <scheidegger.a@gmail.com>

See Also

MCMC, MCMC.parallel

Examples

```
## ----------------------
## Banana shaped distribution

## log-pdf to sample from
p.log <- function(x) {
  B <- 0.03                               # controls 'bananacity'
  -x[1]^2/200 - 1/2*(x[2]+B*x[1]^2-100*B)^2
}


## ----------------------
## generate 200  samples

samp <- MCMC(p.log, n=200, init=c(0, 1), scale=c(1, 0.1),
               adapt=TRUE, acc.rate=0.234, list=TRUE)


## ----------------------
## add 200 to the existing chain
samp <- MCMC.add.samples(samp, n.update=200)

str(samp)
```

`MCMC.parallel` *Parallel computation of MCMC()*

Description

A wrapper function to generate several independent Markov chains by stetting up cluster on a multi-core machine. The function is based on the **parallel** package.

Usage

```
MCMC.parallel(p, n, init, n.chain = 4, n.cpu, packages = NULL, dyn.libs=NULL,
    scale = rep(1, length(init)),  adapt = !is.null(acc.rate),
    acc.rate = NULL, gamma = 2/3, list = TRUE, ...)
```

Arguments

p	function that returns a value proportional to the log probability density to sample from. Alternatively the function can return a list with at least one element named log.density.
n	number of samples.
init	vector with initial values.
n.chain	number of independent chains.
n.cpu	number of CPUs that should be used in parallel.
packages	vector with name of packages to load into each instance. (Typically, all packages on which p depends.)
dyn.libs	vector with name of dynamic link libraries (shared objects) to load into each instance. The libraries must be located in the working directory.
scale	vector with the variances *or* covariance matrix of the jump distribution.
adapt	if TRUE, adaptive sampling is used, if FALSE classic metropolis sampling, if a positive integer the adaption stops after adapt iterations.
acc.rate	desired acceptance rate (ignored if adapt=FALSE)
gamma	controls the speed of adaption. Should be between 0.5 and 1. A lower gamma leads to faster adaption.
list	logical. If TRUE a list of lits is returned otherwise a list of matrices with the samples.
...	further arguments passed to p

Details

This function is just a wrapper to use MCMC in parallel. It is based on **parallel**. Obviously, the application of this function makes only sense on a multi-core machine.

Value

A list with a list or matrix for each chain. See MCMC for details.

Author(s)

Andreas Scheidegger, <andreas.scheidegger@eawag.ch> or <scheidegger.a@gmail.com>

See Also

MCMC

Examples

```
## ----------------------
## Banana shaped distribution

## log-pdf to sample from
p.log <- function(x) {
  B <- 0.03                             # controls 'bananacity'
  -x[1]^2/200 - 1/2*(x[2]+B*x[1]^2-100*B)^2
}

## ----------------------
## generate samples
## compute 4 independent chains on 2 CPU's (if available) in parallel

samp <- MCMC.parallel(p.log, n=200, init=c(x1=0, x2=1),
    n.chain=4, n.cpu=2, scale=c(1, 0.1),
    adapt=TRUE, acc.rate=0.234)

str(samp)
```

Index

adapt_S, *5*
adaptMCMC *(*adaptMCMC-package*)*, 2
adaptMCMC-package, 2

convert.to.coda, *2*, 2

MCMC, *2, 3*, 4, *8, 9*
mcmc, *3*
MCMC.add.samples, *2*, *6*, 7
mcmc.list, *3*
MCMC.parallel, *2*, *6*, *8*, 8