compareMCMCs

an R package for running, managing, and comparing results from different MCMC packages

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Introduction

Markov chain Monte Carlo (MCMC) are methods used to simulate from complicated probability distributions

- Widely used in Bayesian statistical analysis
  ➡️ target distribution: posterior distribution of parameters given data.
- There are many MCMC algorithms (a.k.a. samplers)
  - Metropolis-Hastings (conjugate samplers)
  - Hamiltonian Monte Carlo (HMC)
  - Multivariate samplers
  - ... new methods are constantly developed
- Methods are also implemented differently in different software

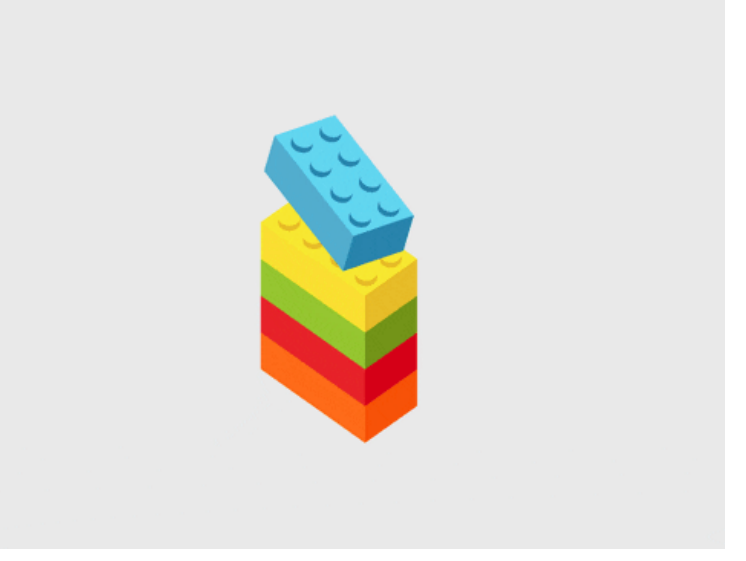


Plenty of possibilities...

- Samplers can be combined

  i.e. use a different algorithm for each parameter

- Implementations of the same algorithm can differ between software packages



Questions

1. Which algorithms are "better" for a given model?
2. Which software implements better an algorithm?

Efficiency in MCMC

Algorithmic mixing & computational speed

- Mixing measured in terms of **Effective Sample Size** (ESS) equivalent number of independent samples
    - R packages implementing different estimators for the ESS
      `coda`, `mcmcse`, `batchmeans`, `stableGR` ...
- Speed
    - sampling time vs total time (e.g. MCMC vs HMC)
    - language of implementation (e.g. R vs C++)

Efficiency = ESS/(time in seconds)

compareMCMCs

Package for managing performance comparisons among MCMC software packages

Features

- the `compareMCMCs` function: run one or more MCMCs and manage the results.
- the `MCMCresult` class to manage results
- a plugin system to include new MCMC engines;
- a plugin system for new metrics for comparison among MCMCs;
- a system for applying parameter conversions, in case difference MCMCs use different parameterizations and/or parameter names;
- a system for generating html pages with figures from comparison metrics, including a plugin system to provide new page components;

Supported software

- Probabilistic programming languages
  ➡️ programming paradigm for automated inference

  - `jags` (`rjags`) - uses mostly on slice samplers
  - `stan` (`rstan`) - Hamiltonian Monte Carlo
  - `nimble` - suite of different algorithms

A toy example

- adaptive M-H with nimble (default)
- slice sampling with nimble

- slice sampling with JAGS (default)
- HMC with Stan (default)

A toy example

```
library(compareMCMCs)
library(nimble)

# This model code will be used for both nimble
# and JAGS
modelCode <- nimbleCode({
    a ~ dunif(0, 100)
    y ~ dgamma(a, 2)
})

modelInfo <- list(code = modelCode, constants = list(y = 2),
    inits = list(a = 1))

# Here is a custom MCMC configuration function
# for nimble
configure_nimble_slice <- function(model) {
    configureMCMC(model, onlySlice = TRUE)
}

res_nimble <- compareMCMCs(modelInfo, MCMCs = c("nimble",
    "nimble_slice"), nimbleMCMCdefs = list(nimble_slice = "configure_nir
    MCMCcontrol = list(inits = list(a = 1), niter = 4000,
        burnin = 200))
```

Define the same model in Stan

```
stan_code <- c("data {real y;}",
               "parameters {real a;}",
               "model {target += uniform_lpdf(a | 0, 100);",
               "       target += gamma_lpdf(y | a, 2);}")

## make two lists to provide stan model and arguments for sampling
stan_model_args <- list(model_code = stan_code)

stan_sampling_args <- list(data = list(y=2),
                           init = list(list(a=1)), # one chain
                           warmup = 200,
                           iter = 2000)
```

Run all models in series

```
res <- compareMCMCs(modelInfo,
                    MCMCs = c('jags',
                              'nimble',       # nimble default
                              'nimble_slice', # nimble slice
                              'stan'),
                    nimbleMCMCdefs =
                      list(nimble_slice = 'configure_nimble_slice'),
                    MCMCcontrol = list(inits = list(a = 1),
                                       niter = 2000,
                                       burnin = 200),
                    externalMCMCinfo = list(stan = list(
                      stan_model_args = stan_model_args,
                      sampling_args = stan_sampling_args)))
```

or combine them later

```
res <- c(res_jags, res_nimble, res_nimble_slice, res_stan)
```

`MCMCresult`

Results are stored in an `R6` class (encapsulate OOP & self-modifiable)

- `MCMC`: optional name for the MCMC method.
- `samples`: matrix of MCMC samples (iteration X parameters)
- `times`: a list of times including elements for setup, burn-in, postburn-in (sampling for recorded samples), and sampling (normally burn-in + postburn-in).
- `metrics`: a list of MCMC performance metrics (ESS, efficency, parameter summaries). Organized `byMCMC`, `byParameter`, `other` (not used)

`make_MCMC_comparison_pages()`

Function to create an html output with comparisons of MCMC results - here an example

Comparison metrics

```
res$nimble$metrics
> $byMCMC
>     MCMC min_efficiency mean_efficiency
> 1 nimble       255278.2        255278.2
> $byParameter
>     MCMC Parameter     mean   median       sd CI95_low CI95_upp
> 1 nimble         a 5.056558 4.931279 2.057118 1.552509 9.306015
>   ESS     efficiency
> 1 765.8347  255278.2
> $other
> list()
```

Add new metrics

Function that takes as input a `MCMCresult` object and outputs a list

```
MCMCmetric_median <- function(result, ...) {
    res <- apply(result$samples, 2, median)
    list(byParameter = list(median = res))
}

addMetrics(res, list(MCMCmetric_median))
```

Page plug-in: figure or text component

A page plug-in is a list with up to five elements:

- `make`: name of a function to create the plottable output such as a ggplot object.
- `fileSuffix`: is a character suffix for figures name
- `linkText`: hyperlink at the top of the comparison page.
- `plot`: name of a function that plot the output to a jpeg file. The function takes as input the `plottable` element of the list returned from `make`.
- `control`: is a list that will be passed to the make function.

Registering the component

```
registerPageComponents(

  list(myNewComponent =
         list(make = "myMakeFunction",
              fileSuffix = "_myPageComponent",
              linkText = "My new page component.")
       )
  )
```

More about `make`

`make` names a function with 2 arguments

1. tidy metrics from `combineMetrics(res, include_times = TRUE)`
2. `control` element of the plugin (user defined)

Return information

1. figure component
   The plotting is done between via call to `jpeg` and `dev.off()`
   - `plottable` - an object that can be plot
   - `height`
   - `width`
2. text component
   - `printable`- character string of html or output from the `xtable` package (that can be plotted as html)

New MCMC plugins

An interface to a new MCMC engine is provided as a function that runs the algorithms and return and `MCMCresult` object

- `MCMCinfo`: The element of `externalMCMCinfo` named to match this MCMC plugin. This can contain whatever information is needed for the plugin.
- `MCMCcontrol`: The `MCMCcontrol` argument to `compareMCMCs`.
- `monitorInfo`: A list of names of parameters to monitor (record) in MCMC output.
- `modelInfo` : The `modelInfo` argument to `compareMCMCs`. If the call to `compareMCMCs` involved creating a `nimble` model, it will be added to this list with the name `model`.

Status

- version of the package on CRAN & Github
  https://cran.r-project.org/web/packages/compareMCMCs/index.html
  https://github.com/nimble-dev/compareMCMCs/tree/master
- Paper on Journal of Open Source Software
  https://joss.theoj.org/papers/10.21105/joss.03844
- Online vignette

Development

- Improve documentation
- Add usage examples
- Any suggestion?