

Package ‘BayesMVP’

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Type Package

Title BayesMVP: A high-performance implementation of adaptive diffusion-space HMC for multivariate probit models and other models with high-dimensional latent variables.

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Description BayesMVP uses diffusion-space Hamiltonian Monte Carlo (HMC) to efficiently sample the multivariate probit model (MVP) to model correlated binary data, as well as the latent class MVP model for the evaluation of test accuracy data without a gold standard. It achieves rapid sampling through manually-derived gradients and chunking. Users can also input any Stan model for efficient sampling of high dimensional latent variable vectors.

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Imports Rcpp (>= 1.0.10), RcppEigen, RcppParallel, dqrng, cmdstanr, bridgestan, bayesplot, posterior, dplyr, ggplot2, tibble, tictoc

LinkingTo Rcpp, RcppEigen, RcppParallel, dqrng

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bridgestan_path	<i>bridgestan_path</i>
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Description

bridgestan_path

Usage

bridgestan_path()

cmdstanr_path	<i>cmdstanr_path</i>
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Description

cmdstanr_path

Usage

cmdstanr_path()

MVP_model	<i>MVP Model Class</i>
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Description

R6 Class for MVP model initialization and sampling.

Details

MVP Model Class

This class handles:

- Model initialization and compilation
- MCMC sampling with adaptive diffusion-pathspace HMC.
- Parameter updates and diagnostics
- Support for both built-in models (MVP, LC-MVP, latent_trait) and user-supplied Stan models

Model Types

- MVP: Multivariate probit model
- LC-MVP: Latent class multivariate probit model
- latent_trait: Latent trait model
- Stan: User-supplied Stan models (files extension must be .stan).

Typical workflow

```
#### NOTE: Please see the ".R" example files for full details & examples,
#### as this is NOT a complete working example, but is provided just to show
#### what order you should call things in.
#### ----- Compile + initialise the model using "MVP_model$new(...)" -----
require(BayesMVP)
## NOTE: The "model_args_list" argument is only needed for BUILT-IN (not Stan) models.
model_obj <- BayesMVP::MVP_model$new(
  Model_type = Model_type,
  y = y,
  N = N,
  model_args_list = model_args_list,
  init_lists_per_chain = init_lists_per_chain,
  sample_nuisance = TRUE,
  n_chains_burnin = n_chains_burnin,
  n_params_main = n_params_main,
  n_nuisance = n_nuisance)

#### --- SAMPLE MODEL: -----
model_samples <- model_obj$sample(
  partitioned_HMC = FALSE,
  diffusion_HMC = FALSE,
  seed = 123,
  n_burnin = 500,
  n_iter = 1000,
  y = y,
  N = N,
  n_params_main = n_params_main,
  n_nuisance = n_nuisance,
  init_lists_per_chain = init_lists_per_chain,
  n_chains_burnin = 8,
  n_chains_sampling = 16,
  model_args_list = model_args_list,
  adapt_delta = 0.80,
  learning_rate = 0.05)

#### --- EXTRACT MODEL RESULTS SUMMARY + DIAGNOSTICS -----
model_fit <- model_samples$summary(
  save_log_lik_trace = FALSE,
  compute_nested_rhat = FALSE,
```

```

compute_transformed_parameters = FALSE)

## extract # divergences +
model_fit$get_divergences()

#### --- TRACE PLOTS -----
## trace_plots_all <- model_samples$plot_traces() # if want the trace for all parameters
trace_plots <- model_fit$plot_traces(
  params = c("beta", "Omega", "p"),
  batch_size = 12)

## you can extract parameters by doing: "trace$param_name()".
## For example:
## display each panel for beta and Omega ("batch_size" controls the # of plots per panel)
trace_plots$beta[[1]] # 1st (and only) panel

#### --- POSTERIOR DENSITY PLOTS -----
## density_plots_all <- model_samples$plot_densities() # if want the densities
## for all parameters.
## Let's plot the densities for: sensitivity, specificity, and prevalence
density_plots <- model_fit$plot_densities(
  params = c("Se_bin", "Sp_bin", "p"),
  batch_size = 12)

## you can extract parameters by doing: "trace$param_name()".
## For example:
## display each panel for beta and Omega ("batch_size" controls the # of plots per panel)
density_plots$Se[[1]] # Se - 1st (and only) panel
density_plots$Sp[[1]] # Sp - 1st (and only) panel
density_plots$p[[1]] # p (prevalence) - 1st (and only) panel

##### --- EXTRACT PARAMETER SUMMARY TIBBLES: -----
## The "model_summary" object (created using the "$summary()" method) contains
## many useful objects.
## For example:
require(dplyr)
## nice summary tibble for main parameters, includes ESS/Rhat, etc:
model_fit$get_summary_main()
## nice summary tibble for transformed parameters, includes ESS/Rhat, etc:
model_fit$get_summary_transformed()
## nice summary tibble for generated quantities, includes
## ESS/Rhat, etc (for LC-MVP this includes Se/Sp/prevalence):
model_fit$get_summary_generated_quantities ()

```

Public fields

Model_type Type of model to fit (can be one of: "MVP", "LC_MVP", "latent_trait" for built-in models, or "Stan" for fitting any Stan model via BayesMVP).

init_object Initialization object.

result Model results object.

model_fit_object Model fit object.

y The dataset. Note that for built-in models (i.e., MVP, LC_MVP, or latent_trait) y should be an $N \times n_{\text{outcomes}}$ matrix.

N The total sample size. Note that for built-in models (i.e., MVP, LC_MVP, or latent_trait) this should be equal to: $N = nrow(y)$.

n_params_main The total number of main model parameters (i.e., excluding nuisance parameters / high-dimensional latent variables). For Stan models (i.e., if "Model_type" is set to "Stan" and you are running a Stan model), this should equal the number of parameters that you define in the "parameters" block of the Stan model, EXCEPT for any nuisance parameters (i.e., high-dimensional latent variables).

n_nuisance The total number of nuisance parameters, i.e. the dimension of the high-dimensional latent variable vector. For built-in models (i.e., MVP, LC_MVP, or latent_trait), this should be equal to: $n_{\text{nuisance}} = N \cdot n_{\text{outcomes}} = nrow(y) \cdot ncol(y)$.

init_lists_per_chain A list of dimension n_chains_burnin (NOT n_chains_sampling, unless n_chains_sampling = n_chains_burnin), where each element of the list is another list which contains the # initial values for the chain. Note that this is the same format for initial values that Stan (both rstan and cmdstanr) uses.

model_args_list List containing model-specific arguments. This is only relevant for built-in models (i.e., MVP, LC_MVP, or latent_trait). All arguments in this list are optional.

Arguments which are relevant to all three of the built-in models include:

- **n_covariates_per_outcome**: A matrix of dimension n_class x n_outcomes, which contains the number of covariates per outcome. If your model has no covariates (which is often the case for the LC_MVP or latent_trait), this does not need to be included, and it just be a matrix of 1's (since each outcome has 1 intercept). Also note that n_class = 1 for the MVP, and for the LC_MVP and latent_trait n_class = 2.
- **prior_coeffs_mean**: An array of dimension n_class x n_outcomes x n_covariates_max, where n_covariates_max is equal to the number of covariates which are contained in the outcome which has the most covariates. This matrix contains the prior mean of each coefficient parameter. In other words, if: $\beta_{c,t,k} \sim N(\mu_{c,t,k}, \sigma_{c,t,k})$, then element (c, t, k) in the matrix corresponds to $\mu_{c,t,k}$, where c is an index for class, t is an index for outcome, and k is an index for the coefficient for outcome t . The default is an array of zeros.
- **prior_coeffs_sd**: This is the same as prior_coeffs_mean, except that each element in the array corresponds to the prior SD. In other words, each element in the array corresponds to: $\sigma_{c,t,k}$, where: $\beta_{c,t,k} \sim N(\mu_{c,t,k}, \sigma_{c,t,k})$. The default is an array of ones.
- **vect_type**: The SIMD (single-instruction, multiple-data) vectorisation type to use for math functions (such as log, exp, Phi, etc). The default is AVX-512 if available, then AVX2 if not, and if neither AVX-512 nor AVX2 are available (e.g., on ARM-based CPU's such as Apple systems), then BayesMVP will use the Stan C++ math library functions, and they will decide what vectorisation type to use. More vectorisation types will be supported in the future.

- `num_chunks`: The number of chunks to use in the log-probability and gradient function. By default, the number selected will depend on your CPU.
- `Phi_type`: Type of $\Phi()$ function implementation to use, where $\Phi()$ is the standard normal CDF. Can be either "Phi" (the default) or "Phi_approx". The default is "Phi". Note that $\Phi()$ will use a fast, highly accurate polynomial approximation of $\Phi()$ if `vect_type` is either AVX-512 or AVX2. Otherwise, it will use the Phi function from the Stan math C++ library.

Arguments which are only relevant to the MVP and LC_MVP include:

- `corr_force_positive`: This will force all elements in the correlation matrix (or matrices if LC_MVP) to be positive. Uses the method proposed by Pinkney et al, 2024.
- `lkj_cholesky_eta`: This is a vector of length `n_class`, where each element corresponds to the LKJ prior parameter η_c corresponding to latent class c . For non-latent class models (i.e., the MVP), this will just be a vector with 1 element e.g. `c(4)` corresponds to: $\Omega \sim \text{LKJ}(4)$. For latent class models (i.e. the LC_MVP and the latent_trait models), the first element corresponds to the first latent class (for test accuracy applications this will be the NON-diseased class) and the second element corresponds to the second latent class (for test accuracy applications this will be the diseased class).
- `ub_corr`: An array of dimension `n_class x n_outcomes x n_outcomes`, which contains the upper-bounds for the correlations. Note that only the lower-triangular elements of each of the supplied `n_class` matrices are used, and the default is a matrix with lower-triangular part all equal to 1.
- `lb_corr`: An array of dimension `n_class x n_outcomes x n_outcomes`, which contains the lower-bounds for the correlations. Note that only the lower-triangular elements of each of the supplied `n_class` matrices are used, and the default is a matrix with lower-triangular part all equal to 0.
- `known_values_indicator`: An array of dimension `n_class x n_outcomes x n_outcomes`, which contains elements that are either 1 or 0, such that: if element (c, t_1, t_2) is 0, then correlation (c, t_1, t_2) is unknown and will be estimated, however if element (c, t_1, t_2) is 1, then we know correlation (c, t_1, t_2) a priori and hence it will be fixed - specifically it will be set equal to the corresponding value in `known_values` (see below). In other words, if any correlations are known a priori, they can be passed onto the model via this argument. Note that only the lower-triangular elements of each of the supplied `n_class` matrices are used, and the default is a matrix with lower-triangular part all equal to 0 (i.e., assumes no # correlations are known/fixed).
- `known_values`: An array of dimension `n_class x n_outcomes x n_outcomes`, which contains any known values for the correlations. In other words, if any correlations are known a priori, they can be passed onto the model via this argument. Note that only the lower-triangular elements of each of the supplied `n_class` matrices are used, and the default is a matrix with lower-triangular part all equal to 0 (note that these values are arbitrary since the elements in `known_values_indicator` are all equal to zero, so they will be ignored unless one or more elements in `known_values_indicator` is non-zero).

Arguments which are only relevant to latent class models (i.e. the LC_MVP and latent_trait models):

- `prev_prior_a`: Shape parameter 1 for prevalence beta prior. Only relevant for latent-class models (i.e. the LC_MVP or latent_trait models).
- `prev_prior_b`: Shape parameter 2 for prevalence beta prior. Only relevant for latent-class models (i.e. the LC_MVP or latent_trait models).

Arguments which are only relevant to the latent trait model (i.e., if `Model_type = "latent_trait"`) include:

- `LT_b_priors_shape`: A matrix of dimension `n_class` x `n_outcomes`, where each element corresponds to the prior Weibull shape parameter of the "b" parameters in the latent trait model - which are denoted as `LT_b`. The default is a matrix with every value equal to 1.33. Please see `LT_b_priors_scale` below for a justification of this default choice.
- `LT_b_priors_scale`: A matrix of dimension `n_class` x `n_outcomes`, where each element corresponds to the prior Weibull scale parameter of the "b" parameters in the latent trait model - which are denoted as `LT_b`. The default is a matrix with every value equal to 1.25. Together with the default choice `LT_b_priors_shape` (please see description above), these priors correspond to the following Weibull priors: $b_{c,t} \sim \text{Weibull}(1.33, 1.250)$. We chose these as default values because they are equivalent to setting truncated-LKJ (1.5) priors in the LC_MVP model, which are very weakly informative, especially if the dimension (i.e. number of outcomes/tests) is small.
- `LT_known_bs_indicator`: A matrix of dimension `n_class` x `n_outcomes`, which contains elements that are either 1 or 0, such that: if element (c, t) is 0, then the corresponding `LT_b` parameter is unknown and will be estimated; however, if element (c, t) is 1, then we know the corresponding `LT_b` parameter a priori and hence it will be fixed - specifically it will be set equal to the corresponding value in `LT_known_bs_values`. In other words, if any `LT_b` are known a priori, they can be passed onto the model via this argument.
- `LT_known_bs_values`: A matrix of dimension `n_class` x `n_outcomes`, which contains any known values for the `LT_b` parameters. In other words, if any `LT_b` are known a priori, they can be passed onto the model via this argument.

`Stan_data_list` List containing data for Stan models (only relevant if "Model_type" is set to "Stan"). The elements of the list should correspond to the variables defined in the "data" block of your Stan model.

`sample_nuisance` Whether or not to sample the high-dimensional nuisance/latent variable vector.

`n_chains_burnin` The total number of burn-in chains. The default is `Min(8, n_cores)`, where `n_cores` is the number of cores on the CPU.

Methods

Public methods:

- `MVP_model$new()`
- `MVP_model$sample()`
- `MVP_model$summary()`
- `MVP_model$clone()`

Method `new()`: Create a new MVP model object

Usage:

```
MVP_model$new(
  Model_type,
  y,
  N,
  n_params_main,
```

```

    n_nuisance,
    init_lists_per_chain,
    n_chains_burnin,
    compile = TRUE,
    force_recompile = TRUE,
    model_args_list = NULL,
    Stan_data_list = NULL,
    sample_nuisance = NULL,
    Stan_model_file_path = NULL,
    Stan_cpp_user_header = NULL,
    Stan_cpp_flags = NULL,
    ...
)

```

Arguments:

Model_type Type of model ("MVP", "LC-MVP", etc.). See class documentation for details.

y The dataset. See class documentation for details.

N The sample size. See class documentation for details.

n_params_main Number of main parameters. See class documentation for details.

n_nuisance Number of nuisance parameters. See class documentation for details.

init_lists_per_chain List of initial values for each chain. See class documentation for details.

n_chains_burnin Number of chains used for burnin. See class documentation for details.

compile Compile the (possibly dummy if using built-in models) Stan model.

force_recompile Force-compile the (possibly dummy if using built-in models) Stan model.

model_args_list List of model arguments. See class documentation for details.

Stan_data_list List of Stan data (optional). See class documentation for details.

sample_nuisance Whether to sample nuisance parameters. See class documentation for details.

Stan_model_file_path The file path to the Stan model, only needed if **Model_type** = "Stan".

Stan_cpp_user_header The file path to a user-supplied C++ .hpp file to be compiled together with the Stan model. This is optional and only needed if you want to use custom C++ functions in your Stan model, and is only relevant if **Model_type** = "Stan".

Stan_cpp_flags User-supplied R list containing comma-separated values of compiler flags (e.g. CXX_FLAGS, etc) to be passed on to cmdstanr - the Stan model will then be compiled using these flags. This is optional and only needed if you want to use custom C++ functions in your Stan model. Only relevant if **Model_type** = "Stan".

... Additional arguments passed to `BayesMVP::initialise_model`.

Returns: Returns `self$init_object`, an object generated from the "BayesMVP::initialise_model" function which contains information such as which model type (**Model_type**) to use.

Method `sample()`: Sample from the model

Usage:

```

MVP_model$sample(
  init_lists_per_chain = self$init_lists_per_chain,
  model_args_list = self$model_args_list,

```



```

Stan_data_list = self$Stan_data_list,
parallel_method = "RcppParallel",
y = self$y,
N = self$N,
manual_tau = NULL,
tau_if_manual = NULL,
sample_nuisance = self$sample_nuisance,
partitioned_HMC = FALSE,
diffusion_HMC = FALSE,
vect_type = NULL,
Phi_type = "Phi",
n_params_main = self$n_params_main,
n_nuisance = self$n_nuisance,
n_chains_burnin = self$n_chains_burnin,
n_chains_sampling = NULL,
n_superchains = NULL,
seed = NULL,
n_burnin = 500,
n_iter = 1000,
adapt_delta = 0.8,
learning_rate = NULL,
clip_iter = NULL,
interval_width_main = NULL,
interval_width_nuisance = NULL,
force_autodiff = FALSE,
force_PartialLog = FALSE,
multi_attempts = TRUE,
max_L = 1024,
tau_mult = 1.6,
metric_type_main = "Hessian",
metric_shape_main = "diag",
metric_type_nuisance = "Empirical",
ratio_M_main = 0.25,
ratio_M_us = 0.25,
force_recompile = FALSE,
...
)

```

Arguments:

`init_lists_per_chain` List of initial values for each chain. See class documentation for details.

`model_args_list` List of model arguments. See class documentation for details.

`Stan_data_list` List of Stan data (optional). See class documentation for details.

`parallel_method` The method to use for parallelisation (multithreading) in C++. Default is "RcppParallel". Can be changed to "OpenMP", if available.

`y` The dataset. See class documentation for details.

`N` The sample size. See class documentation for details.

`manual_tau` If FALSE, then SNAPER-HMC will be used to adapt τ during the burnin phase. Otherwise if TRUE, τ will be fixed to the value given in the `tau_if_manual` argument.

- tau_if_manual** The HMC path length (τ) to use for the HMC sampling. This will be used for both the burnin and sampling phases. Note that this only works if `manual_tau = TRUE`. Otherwise, τ will be adapted using SNAPER-HMC. Also note that if only one value is given, then this value of tau will be used for both the main parameter sampling and the nuisance parameter sampling. If you want to specify separate path lengths for the main and nuisance parameters, provide a vector instead. E.g. `tau_if_manual = c(0.50, 2.0)` will mean that $\tau = 0.50$ is used for the main parameters and $\tau = 2.0$ is used for the nuisance parameters.
- sample_nuisance** Whether to sample nuisance parameters. See class documentation for details.
- partitioned_HMC** Whether to sample all parameters at once (note: wont use diffusion HMC) or whether to alternate between sampling the nuisance parameters and the main model parameters.
- diffusion_HMC** Whether to use diffusion-pathsapce HMC (Beskos et al) to sample nuisance parameters. Default is TRUE.
- vect_type** The SIMD (single-nstruction, multiple-data) vectorisation type to use for math functions (such as log, exp, Phi, etc). The default is AVX-512 if available, then AVX2 if not, and if neither AVX-512 nor AVX2 are available (e.g., on ARM-based CPU's such as Apple systems), then BayesMVP will use the Stan C++ math library functions, and they will decide what vectorisation type to use. More vectorisation types will be supported in the future.
- Phi_type** Type of Phi() function implementation to use, where Phi() is the standard normal CDF. Can be either "Phi" (the default) or "Phi_approx()".
- n_params_main** Number of main parameters. See class documentation for details.
- n_nuisance** Number of nuisance parameters. See class documentation for details.
- n_chains_burnin** Number of chains used for burnin. See class documentation for details.
- n_chains_sampling** Number of chains used for sampling (i.e., post-burnin). Note that this must match the length of "init_lists_per_chain".
- n_superchains** Number of superchains for nested R-hat (nR-hat; see Margossian et al, 2023) computation.
- seed** Random MCMC seed.
- n_burnin** The number of burnin iterations. Default is 500.
- n_iter** The number of sampling (i.e., post-burnin) iterations. Default is 1000.
- adapt_delta** The Metropolis-Hastings target acceptance rate. Default is 0.80. If there are divergences, sometimes increasing this can help, at the cost of efficiency (since this will decrease the step-size (epsilon) and increase the number of leapfrog steps (L) per iteration).
- learning_rate** The ADAM learning rate (LR) for learning the appropriate HMC step-size (ϵ) and HMC path length ($\tau = L \cdot \epsilon$) during the burnin period. The default depends on the length of burnin chosen as follows: if `n_burnin < 249`, then LR=0.10, if it's between 250 and 500 then LR = 0.075, and if the burnin length is between 501 and 750 then LR=0.05, and finally if the burnin is >750 iterations then LR=0.025.
- clip_iter** The number of iterations to perform MALA (i.e., one leapfrog step) on (first clip_iter iterations) for the burnin period. The default depends on the length of the burnin period.
- interval_width_main** How often to update the metric (which is either empirical or Hessian-informed, and can be diagonal or dense) for the main parameters during the burnin period. The default used depends on the length of the burnin period.

interval_width_nuisance How often to update the metric (which is empirical and diagonal) for the nuisance parameters during the burnin period. The default used depends on the length of the burnin period.

force_autodiff Whether to use (force) autodiff instead of the built-in manual gradients. This is only relevant for the built-in models, not Stan models. The default is FALSE.

force_PartialLog Whether to use (force) use of gradients on the log-scale (for stability). Note that if `force_autodiff = TRUE` then this will automatically be set to TRUE, since autodiff is only available for partial-log-scale gradients. The default is FALSE.

multi_attempts Whether

max_L The maximum number of leapfrog steps. This is similar to `max_treedepth` in Stan. The default is 1024 (which is equivalent to the default `max_treedepth = 10` in Stan).

tau_mult The SNAPER-HMC algorithm multiplier to use when adjusting the path length during the burnin phase.

metric_type_main The type of metric to use for the main parameters, which is adapted during the burnin period. Can be either "Hessian" or "Empirical", where the former uses second derivative information and the latter uses the SD of the posterior computed whilst sampling. The default is "Hessian" if `n_params_main < 250` and "Empirical" otherwise.

metric_shape_main The shape of the metric to use for the main parameters, which is adapted during the burnin period. Can be either "diag" or "dense". The default is "diag" (i.e. a diagonal metric).

metric_type_nuisance The type of metric to use for the nuisance parameters, which is adapted during the burnin period. Can be "diag" or "unit".

ratio_M_main Ratio to use for the metric. Main parameters.

ratio_M_us Ratio to use for the metric. Nuisance parameters.

force_recompile Recompile the (possibly dummy if using built-in model) Stan model.

... Additional arguments passed to sampling.

Returns: Returns self invisibly, allowing for method chaining of this classes (MVP_model) methods. E.g.: `model$sample(...)$summary(...)`.

Method summary(): Create and compute summary statistics, traces and model diagnostics.

Usage:

```
MVP_model$summary(
  compute_main_params = TRUE,
  compute_transformed_parameters = TRUE,
  compute_generated_quantities = TRUE,
  save_log_lik_trace = TRUE,
  save_nuisance_trace = FALSE,
  compute_nested_rhat = NULL,
  n_superchains = NULL,
  save_trace_tibbles = FALSE,
  ...
)
```

Arguments:

compute_main_params Whether to compute the main parameter summaries. Default is TRUE. Note that this excludes the high-dimensional nuisance parameter vector (for Stan models -

this should be defined as the FIRST parameter in the "parameters" block). For Stan models, this will be for the parameters defined the "parameters" block of the model. For built-in models (i.e. the MVP, LC_MVP, and latent_trait), this will compute summaries and traces for the coefficient vector (beta; for all 3 models), the correlation matrix/matrices (Omega; for the MVP and LC_MVP only), for the latent_trait latent effect coefficients (i.e. the "b" parameters - denoted "LT_b" - for latent_trait only), and finally for the disease prevalence ("p" or "prev"; for the LC_MVP and latent_trait only).

`compute_transformed_parameters` Whether to compute transformed parameter summaries. Default is TRUE. For Stan models, this will be for all of the parameters defined in the "transformed parameters" block, EXCEPT for the (transformed) nuisance parameters and `log_lik` (see "save_log_lik_trace" for more information on `log_lik`).

`compute_generated_quantities` Whether to compute the summaries for generated quantities. Default is TRUE. For Stan models this will exclude any `log_lik` defined in the "generated quantities" block - see "save_log_lik_trace".

`save_log_lik_trace` Whether to save the log-likelihood (`log_lik`) trace. Default is FALSE. For Stan models, this will only work if there is a "log_lik" parameter defined in the "transformed parameters" model block. For built-in models,

`save_nuisance_trace` Whether to save the nuisance trace. Default is FALSE.

`compute_nested_rhat` Whether to compute the nested rhat diagnostic (nR-hat) (Margossian et al, 2023). This is useful when running many (usually short) chains. Also see "n_superchains" argument.

`n_superchains` The number of superchains to use for the computation of nR-hat. Only relevant if `compute_nested_rhat` = TRUE.

`save_trace_tibbles` Whether to save the trace as tibble dataframes as well as 3D arrays. Default is FALSE.

... Any other arguments to be passed to `BayesMVP::create_summary_and_traces`.

Returns: Returns a new MVP_plot_and_diagnose object (from the "MVP_plot_and_diagnose" R6 class) for creating MCMC diagnostics and plots.

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

```
MVP_model$clone(deep = FALSE)
```

Arguments:

`deep` Whether to make a deep clone.

MVP_plot_and_diagnose *MVP extract and plot Class*

Description

Class for handling MVP model summaries, samples (trace) and diagnostics.

Details

This class is called via the main "MVP_model" R6 class.

Model Types

- MVP: Multivariate probit model
- LC-MVP: Latent class multivariate probit model
- latent_trait: Latent trait model
- Stan: User-supplied Stan models (files extension must be .stan).

Class Relationship

This class is not meant to be instantiated/called directly by users. Instead, it is created and returned by the MVP_model\$summary() method. It provides methods for:

- Extracting MCMC diagnostics (divergences, ESS, etc.)
- Creating trace and density plots
- Computing efficiency metrics
- Accessing posterior draws in various formats

Common Usage Patterns

Basic Diagnostics get_divergences() -> get_efficiency_metrics()

Parameter Summaries get_summary_main() -> get_summary_transformed()

Visualization plot_traces() -> plot_densities()

Custom Analysis get_posterior_draws() -> Your analysis

Public fields

summary_object The summary object, obtained from the main "MVP_model" R6 class.

init_object Initialization object, obtained from the main "MVP_model" R6 class.

n_nuisance The total number of nuisance parameters, please see the "MVP_model" R6 class documentation for more details.

Methods

Public methods:

- MVP_plot_and_diagnose\$new()
- MVP_plot_and_diagnose\$get_divergences()
- MVP_plot_and_diagnose\$get_summary_main()
- MVP_plot_and_diagnose\$get_summary_transformed()
- MVP_plot_and_diagnose\$get_summary_generated_quantities()
- MVP_plot_and_diagnose\$get_posterior_draws()
- MVP_plot_and_diagnose\$get_all_traces()
- MVP_plot_and_diagnose\$get_log_lik_trace()
- MVP_plot_and_diagnose\$get_nuisance_trace()
- MVP_plot_and_diagnose\$get_posterior_draws_as_tibbles()
- MVP_plot_and_diagnose\$get_efficiency_metrics()

- `MVP_plot_and_diagnose$get_HMC_info()`
- `MVP_plot_and_diagnose$time_to_target_ESS()`
- `MVP_plot_and_diagnose$iter_to_target_ESS()`
- `MVP_plot_and_diagnose$plot_traces()`
- `MVP_plot_and_diagnose$plot_densities()`
- `MVP_plot_and_diagnose$clone()`

Method new():*Usage:*`MVP_plot_and_diagnose$new(model_summary, init_object, n_nuisance)`*Arguments:*`model_summary` The summary object, obtained from the main "MVP_model" R6 class.`init_object` The Initialization object, obtained from the main "MVP_model" R6 class.`n_nuisance` The total number of nuisance parameters, please see the "MVP_model" R6 class documentation for more details.**Method get_divergences():***Usage:*`MVP_plot_and_diagnose$get_divergences()`

Returns: Returns `self$summary_object$summaries$divergences` obtained from the main "MVP_model" R6 class. `self$summary_object$summaries$divergences` contains divergence information (e.g. % of transitions which diverged).

Method get_summary_main():*Usage:*`MVP_plot_and_diagnose$get_summary_main()`*Returns:* Returns main parameter summaries as a tibble.**Method get_summary_transformed():***Usage:*`MVP_plot_and_diagnose$get_summary_transformed()`*Returns:* Returns transformed parameter summaries as a tibble.**Method get_summary_generated_quantities():***Usage:*`MVP_plot_and_diagnose$get_summary_generated_quantities()`*Returns:* Returns generated quantities as a tibble. Convenience method for posterior draws (as 3D arrays)**Method get_posterior_draws():***Usage:*`MVP_plot_and_diagnose$get_posterior_draws()`*Returns:* Returns posterior draws as a 3D array (iterations, chains, parameters). Convenience method for all traces (as 3D arrays)

Method get_all_traces():*Usage:*

MVP_plot_and_diagnose\$get_all_traces()

Returns: Returns posterior traces as a 3D arrays (iterations, chains, parameters). Convenience method for posterior draws for log_lik (as 3D arrays)**Method** get_log_lik_trace():*Usage:*

MVP_plot_and_diagnose\$get_log_lik_trace()

Returns: Returns posterior draws for log_lik as a 3D array (iterations, chains, parameters). Convenience method for posterior draws for nuisance (as 3D arrays)**Method** get_nuisance_trace():*Usage:*

MVP_plot_and_diagnose\$get_nuisance_trace()

Returns: Returns posterior draws for nuisance as a 3D array (iterations, chains, parameters). Convenience method for posterior draws (as tibbles)**Method** get_posterior_draws_as_tibbles():*Usage:*

MVP_plot_and_diagnose\$get_posterior_draws_as_tibbles()

Returns: Returns trace as tibbles. The trace gets returned as 3 separate tibbles (one tibble for the main parameters, one for the transformed parameters, and one for generated quantities).**Method** get_efficiency_metrics():*Usage:*

MVP_plot_and_diagnose\$get_efficiency_metrics()

Returns: Returns a list containing efficiency metrics including:

- time_burnin: Time spent in burnin phase
- time_sampling: Time spent sampling
- time_total_MCMC: Total time spent doing MCMC/HMC sampling, excluding time to compute summaries and diagnostics.
- time_total_inc_summaries: Total time spent doing MCMC/HMC sampling, including time to compute summaries and diagnostics.
- Min_ESS_main: The minimum ESS of the main model parameters.
- Min_ESS_per_sec_sampling: The minimum ESS per second for the sampling phase.
- Min_ESS_per_sec_total: The minimum ESS per second for the total model run time, including any time spent computing summaries and diagnostics.
- Min_ESS_per_grad_sampling: The minimum ESS per gradient evaluation for the sampling phase.
- grad_evals_per_sec: The number of gradient evaluations performed per second.
- est_time_to_100_ESS_sampling: The estimated sampling time to reach a minimum ESS of 100.

- `est_time_to_1000_ESS_sampling`: The estimated sampling time to reach a minimum ESS of 1000.
- `est_time_to_10000_ESS_sampling`: The estimated sampling time to reach a minimum ESS of 10,000.
- `est_time_to_100_ESS_wo_summaries`: The estimated total time (excluding time to compute model summaries and diagnostics) to reach a minimum ESS of 100.
- `est_time_to_1000_ESS_wo_summaries`: The estimated total time (excluding time to compute model summaries and diagnostics) to reach a minimum ESS of 1000.
- `est_time_to_10000_ESS_wo_summaries`: The estimated total time (excluding time to compute model summaries and diagnostics) to reach a minimum ESS of 10,000.
- `est_time_to_100_ESS_inc_summaries`: The estimated total time (including time spent computing model summaries and diagnostics) to reach a minimum ESS of 100.
- `est_time_to_1000_ESS_inc_summaries`: The estimated total time (including time spent computing model summaries and diagnostics) to reach a minimum ESS of 1000.
- `est_time_to_10000_ESS_inc_summaries`: The estimated total time (including time spent computing model summaries and diagnostics) to reach a minimum ESS of 10,000.

Method `get_HMC_info()`:

Usage:

`MVP_plot_and_diagnose$get_HMC_info()`

Returns: Returns a list containing HMC algorithm metrics including:

- `tau_main`: The HMC path length (τ) for sampling the main parameters.
- `eps_main`: The HMC step-size (ϵ) for sampling the main parameters.
- `tau_us`: The HMC path length (τ) for sampling the nuisance parameters.
- `eps_us`: The HMC step-size (ϵ) for sampling the nuisance parameters.
- `n_chains_sampling`: The number of parallel chains used during the sampling phase.
- `n_chains_burnin`: The number of parallel chains used during the burnin phase.
- `n_iter`: The number of iterations used during the sampling phase.
- `n_burnin`: The number of iterations used during the burnin phase.
- `LR_main`: The ADAM learning rate (main parameters).
- `LR_us`: The ADAM learning rate (nuisance parameters).
- `adapt_delta`: The target Metropolis-Hastings acceptance probability.
- `metric_type_main`: The type of HMC metric used for main parameters (Hessian or Empirical).
- `metric_shape_main`: The shape of HMC metric used for main parameters (dense or diag).
- `metric_type_nuisance`: The type of HMC metric used for the nuisance parameters (Hessian or Empirical).
- `metric_shape_nuisance`: The shape of HMC metric used for the nuisance parameters (dense or diag).
- `diffusion_HMC`: Whether diffusion HMC was used to sample the nuisance parameters or not.
- `partitioned_HMC`: Whether partitioned HMC was used or not (if FALSE, then parameters were sampled all at once, and if TRUE, then the nuisance are sampled conditional on the main parameters).

- `n_superchains`: The number of superchains.
- `interval_width_main`: The interval width for the main parameters. The metric is computed at the end of each interval.
- `interval_width_nuisance`: The interval width for the nuisance parameters. The metric is computed at the end of each interval.
- `force_autodiff`: Whether autodiff was used (forced) - only relevant for built-in models, as Stan models always use autodiff.
- `force_PartialLog`: Whether a partial-log-scale version of the model was used (forced) - only relevant for built-in models.
- `multi_attempts`: Whether multiple attempts were made when evaluating the `lp_grad` function (i.e. first try normal param., then partial-log-scale, and finally autodiff + partial-log-scale) - only relevant for built-in models.

Method `time_to_target_ESS()`:

Usage:

```
MVP_plot_and_diagnose$time_to_target_ESS(target_ESS)
```

Arguments:

`target_ESS` The target ESS.

Returns: Returns a list called "target_ESS_times" which contains the estimated sampling time to reach the target ESS ("`sampling_time_to_target_ESS`"), the estimated total time excluding the time it takes to compute model summaries ("`total_time_to_target_ESS_wo_summaries`"), and the total estimated time to reach the target ESS ("`total_time_to_target_ESS_with_summaries`").

Method `iter_to_target_ESS()`:

Usage:

```
MVP_plot_and_diagnose$iter_to_target_ESS(target_ESS)
```

Arguments:

`target_ESS` The target ESS.

Returns: Returns a list called "target_ESS_iter" which contains the estimated number of sampling iterations (`n_iter`) to reach the target ESS ("`sampling_iter_to_target_ESS`").

Method `plot_traces()`:

Usage:

```
MVP_plot_and_diagnose$plot_traces(params = NULL, batch_size = 9)
```

Arguments:

`params` The parameters to generate trace plots for. This is a character vector - e.g. to plot trace plots for beta: `params = c("beta")`. The default is `NULL` and the trace plots for all model parameters (which have a trace array) will be plotted.

`batch_size` The number of trace plots to display per panel. Default is 9.

Returns: If no parameters specified (i.e. `params = NULL`), then this will return an object containing the trace plots for all model parameters which have a trace array.

Method `plot_densities()`:

Usage:

```
MVP_plot_and_diagnose$plot_densities(params = NULL, batch_size = 9)
```

Arguments:

params The parameters to generate posterior density plots for. This is a character vector - e.g. to plot the posterior density plots for beta: `params = c("beta")`. The default is `NULL` and the posterior density plots for all model parameters (which have a trace array) will be plotted.

batch_size The number of posterior density plots to display per panel. Default is 9.

Returns: If no parameters specified (i.e. `params = NULL`), then this will return an object containing the posterior density plots for all model parameters which have a trace array.

Method `clone()`: The objects of this class are cloneable with this method.

Usage:

```
MVP_plot_and_diagnose$clone(deep = FALSE)
```

Arguments:

deep Whether to make a deep clone.

```
set_pkg_example_path_and_wd
```

```
set_pkg_example_path_and_wd
```

Description

```
set_pkg_example_path_and_wd
```

Usage

```
set_pkg_example_path_and_wd()
```

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