

Package: graDiEnt (via r-universe)

August 21, 2024

Title Stochastic Quasi-Gradient Differential Evolution Optimization

Version 1.1.0

Description An optim-style implementation of the Stochastic Quasi-Gradient Differential Evolution (SQG-DE) optimization algorithm first published by Sala, Baldanzini, and Pierini (2018; <[doi:10.1007/978-3-319-72926-8_27](https://doi.org/10.1007/978-3-319-72926-8_27)>). This optimization algorithm fuses the robustness of the population-based global optimization algorithm "Differential Evolution" with the efficiency of gradient-based optimization. The derivative-free algorithm uses population members to build stochastic gradient estimates, without any additional objective function evaluations. Sala, Baldanzini, and Pierini argue this algorithm is useful for 'difficult optimization problems under a tight function evaluation budget.' This package can run SQG-DE in parallel and sequentially.

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URL <https://github.com/bmgaldo/graDiEnt>

BugReports <https://github.com/bmgaldo/graDiEnt/issues>

Encoding UTF-8

Depends R (>= 3.5.0)

Imports stats, doParallel

Roxygen list(markdown = TRUE)

RoxygenNote 7.3.2

Suggests testthat (>= 3.0.0)

Config/testthat/edition 3

Repository <https://bmgaldo.r-universe.dev>

RemoteUrl <https://github.com/bmgaldo/gradient>

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GetAlgoParams	<i>GetAlgoParams</i>
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Description

Get control parameters for optim_SQGDE function.

Usage

```
GetAlgoParams(
    n_params,
    n_particles = NULL,
    n_diff = 2,
    n_iter = 1000,
    init_sd = 0.01,
    init_center = 0,
    n_cores_use = 1,
    step_size = NULL,
    jitter_size = 1e-06,
    crossover_rate = 1,
    parallel_type = "none",
    return_trace = FALSE,
    thin = 1,
    purify = Inf,
    adapt_scheme = NULL,
    give_up_init = 100,
    stop_check = 10,
    stop_tol = 1e-04,
    converge_crit = "stdev",
    var_list = NULL,
    message_int = 100
)
```

Arguments

n_params	The number of parameters estimated/optimized, this integer value NEEDS to be specified.
n_particles	The number of particles (population size), 3*n_params is the default value.
n_diff	The number of mutually exclusive vector pairs to stochastically approximate the gradient.

<code>n_iter</code>	The number of iterations to run the algorithm, 1000 is default.
<code>init_sd</code>	A positive scalar or <code>n_params</code> -dimensional numeric vector, determines the standard deviation of the Gaussian initialization distribution. The default value is 0.01.
<code>init_center</code>	A scalar or <code>n_params</code> -dimensional numeric vector, determines the mean of the Gaussian initialization distribution. The default value is 0.
<code>n_cores_use</code>	An integer specifying the number of cores used when using parallelization. The default value is 1.
<code>step_size</code>	A positive scalar, jump size or "F" in the DE crossover step notation. The default value is $2.38/\sqrt{2*n_params}$.
<code>jitter_size</code>	A positive scalar that determines the jitter (noise) size. Noise is added during adaption step from Uniform(-jitter_size,jitter_size) distribution. $1e-6$ is the default value. Set to 0 to turn off jitter.
<code>crossover_rate</code>	A numeric scalar on the interval (0,1]. Determines the probability a parameter on a chain is updated on a given crossover step, sampled from a Bernoulli distribution. The default value is 1.
<code>parallel_type</code>	A character string specifying parallelization type. 'none', 'FORK', or 'PSOCK' are valid values. 'none' is default value. 'FORK' does not work with Windows OS.
<code>return_trace</code>	A boolean, if true, the function returns particle trajectories. This is helpful for assessing convergence or debugging model code. The trace will be an iteration/thin \times <code>n_particles</code> \times <code>n_params</code> array containing parameter values and an iteration/thin \times <code>n_particles</code> array containing particle weights.
<code>thin</code>	A positive integer. Only every 'thin'-th iteration will be stored in memory. The default value is 1. Increasing thin will reduce the memory required when running the algorithm for longer.
<code>purify</code>	A positive integer. On every 'purify'-th iteration the particle weights are recomputed. This is useful if the objective function is stochastic/noisy. If the objective function is deterministic, this computation is redundant. Purify is set to Inf by default, disabling it.
<code>adapt_scheme</code>	A character string that must be 'rand', 'current', or 'best' that determines the DE adaption scheme/strategy. 'rand' uses rand/1/bin DE-like scheme where a random particle and the particle-based quasi-gradient approximation are used to generate proposal updates for a given particle. 'current' uses current/1/bin, and 'best' uses best/1/bin which follow an analogous adaption scheme to rand. 'rand' is the default value.
<code>give_up_init</code>	An integer for how many failed initialization attempts before stopping the optimization routine. 100 is the default value.
<code>stop_check</code>	An integer for how often to check the convergence criterion. The default is 10 iterations.
<code>stop_tol</code>	A convergence metric must be less than value to be labeled as converged. The default is $1e-4$.
<code>converge_crit</code>	A character string denoting the convergence metric used, valid metrics are 'stdev' (standard deviation of population weight in the last stop_check iterations) and

	'percent' (percent improvement in median particle weight in the last stop_check iterations). 'stdev' is the default.
var_list	A vector of names of variables and functions to export for parallelization (via parallel::clusterExport). Default value is NULL.
message_int	An integer specifying the interval at which an update message is displayed, based on the number of completed iterations. Must be a positive value. The default is 100; set to Inf to disable these particular messages.

Value

A list of control parameters for the optim_SQGDE function.

optim_SQGDE	<i>optim_SQGDE</i>
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Description

Runs Stochastic Quasi-Gradient Differential Evolution (SQG-DE; Sala, Baldanzini, and Pierini, 2018) to minimize an objective function $f(x)$. To maximize a function $f(x)$, simply pass $g(x)=-f(x)$ to ObjFun argument.

Usage

```
optim_SQGDE(ObjFun, control_params = GetAlgoParams(), ...)
```

Arguments

ObjFun	A scalar-returning function to minimize whose first argument is a real-valued n_{params} -dimensional vector.
control_params	control parameters for SQG-DE algo. see GetAlgoParams function documentation for more details. The only argument you NEED to pass here is n_{params} .
...	additional arguments to pass ObjFun.

Value

list containing solution and it's corresponding weight (i.e. $f(\text{solution})$).

Examples

```
#####
# Maximum Likelihood Example
#####

# simulate from model
dataExample=matrix(rnorm(1000,c(-1,1,0,1),c(1,1,1,1)),ncol=4,byrow = TRUE)

# list parameter names
```

```

param_names_example=c("mu_1", "mu_2", "mu_3", "mu_4")

# negative log likelihood
ExampleObjFun=function(x,data,param_names){
  out=0

  names(x) <- param_names

  # log likelihoods
  out=out+sum(dnorm(data[,1],x["mu_1"],sd=1,log=TRUE))
  out=out+sum(dnorm(data[,2],x["mu_2"],sd=1,log=TRUE))
  out=out+sum(dnorm(data[,3],x["mu_3"],sd=1,log=TRUE))
  out=out+sum(dnorm(data[,4],x["mu_4"],sd=1,log=TRUE))

  return(out*-1)
}

#####
# run optimization
out <- optim_SQGDE(ObjFun = ExampleObjFun,
                  control_params = GetAlgoParams(n_params = length(param_names_example),
                                                n_iter = 250,
                                                n_particles = 12,
                                                n_diff = 2,
                                                return_trace = TRUE),
                  data = dataExample,
                  param_names = param_names_example)
old_par <- par() # save graphic state for user
# plot particle trajectory

par(mfrow=c(2,2))
matplot(out$particles_trace[, ,1],type='l')
matplot(out$particles_trace[, ,2],type='l')
matplot(out$particles_trace[, ,3],type='l')
matplot(out$particles_trace[, ,4],type='l')

#SQG DE solution
out$solution

#analytic solution
apply(dataExample, 2, mean)

par(old_par) # restore user graphic state

```

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