

Package ‘activegp’

April 24, 2020

Type Package

Title Gaussian Process Based Design and Analysis for the Active Subspace Method

Version 1.0.4

Date 2020-04-05

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Description The active subspace method is a sensitivity analysis technique that finds important linear combinations of input variables for a simulator. This package provides functions allowing estimation of the active subspace without gradient information using Gaussian processes as well as sequential experimental design tools to minimize the amount of data required to do so. Implements Wycoff et al. (2019) <arXiv:1907.11572>.

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Depends R (>= 3.4.0)

Imports Rcpp (>= 0.12.18), hetGP (>= 1.1.1), lhs, numDeriv, methods

LinkingTo Rcpp, RcppArmadillo

RoxygenNote 7.1.0

Suggests testthat

NeedsCompilation yes

Repository CRAN

Date/Publication 2020-04-24 04:20:02 UTC

R topics documented:

activegp	2
C_GP	4
C_GP_ci	5
C_tr	6
C_var	8
C_var2	9
domain_to_R	10

domain_to_unit	11
grad_est_subspace	11
logLikHessian	12
n11_2_01	13
print.const_C	13
subspace_dist	14
update.const_C	14
update_C2	15

Index	17
--------------	-----------

activegp	<i>Package activegp</i>
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Description

Active subspace estimation with Gaussian processes

Details

The primary function for analysis of the active subspace given some set of function evaluations is `C_GP`.

`C_var`, `C_var2`, and `C_tr` give three possible acquisition functions for sequential design. Either `C_var` or `C_var2` is recommended, see Wycoff et al for details and the example below for usage.

Author(s)

Nathan Wycoff, Mickael Binois

References

N. Wycoff, M. Binois, S. Wild (2019+), Sequential Learning of Active Subspaces, preprint.
 P. Constantine (2015) Active Subspaces: Emerging Ideas for Dimension Reduction in Parameter Studies, SIAM Spotlights

Examples

```
#####
### Sequential learning of active subspaces
#####
library(hetGP); library(lhs)
set.seed(42)

nvar <- 2
n <- 20
nits <- 20

# theta gives the subspace direction
```

```

f <- function(x, theta, nugget = 1e-6){
  if(is.null(dim(x))) x <- matrix(x, 1)
  xact <- cos(theta) * x[,1] - sin(theta) * x[,2]
  return(hetGP::f1d(xact) + rnorm(n = nrow(x), sd = rep(nugget, nrow(x))))
  return(100*erf((xact + 0.5)*5) + hetGP::f1d(xact) +
    rnorm(n = nrow(x), sd = rep(nugget, nrow(x))))
}

theta_dir <- pi/6
act_dir <- c(cos(theta_dir), -sin(theta_dir))

# Create design of experiments and initial GP model
design <- X <- matrix(signif(maximinLHS(n, nvar), 2), ncol = nvar)
response <- Y <- apply(design, 1, f, theta = theta_dir)
model <- mleHomGP(design, response, lower = rep(1e-4, nvar),
  upper = rep(0.5, nvar), known = list(g = 1e-6, beta0 = 0))

C_hat <- C_GP(model)

ngrid <- 51
xgrid <- seq(0, 1, ngrid)
Xgrid <- as.matrix(expand.grid(xgrid, xgrid))
filled.contour(matrix(f(Xgrid, theta = theta_dir), ngrid))
ssd <- rep(NA, nits)

# Main loop
for(nit in 1:nits) {
  cat(nit)
  cat(" ")

  af <- function(x, C) C_var(C, x, grad = FALSE)
  af_gr <- function(x, C) C_var(C, x, grad = TRUE)
  Ctr_grid <- apply(Xgrid, 1, af, C = C_hat) # CVAR

  # Best candidate point
  opt_cand <- matrix(Xgrid[which.max(Ctr_grid),], 1)

  # Refine with gradient based optimization
  opt <- optim(opt_cand, af, af_gr, method = 'L-BFGS-B', lower = rep(0, nvar), C = C_hat,
    upper = rep(1, nvar), hessian = TRUE,
    control = list(fnscale=-1, trace = 0, maxit = 10))

  # Criterion surface with best initial point and corresponding local optimum
  filled.contour(matrix(Ctr_grid, ngrid), color.palette = terrain.colors,
    plot.axes = {axis(1); axis(2); points(X, pch = 20);
      points(opt_cand, pch = 20, col = 'blue');
      points(opt$par, pch = 20, col = 'red')}})

  X <- rbind(X, opt$par)
  Ynew <- f(opt$par, theta = theta_dir)
  Y <- c(Y, Ynew)
  model <- update(model, Xnew = opt$par, Znew = Ynew)
}

```

```

## periodically restart model fit
if(nit %% 5 == 0){
mod2 <- mleHomGP(X = list(X0 = model$X0, Z0 = model$Z0, mult = model$mult), Z = model$Z,
                 known = model$used_args$known, lower = model$used_args$lower,
                 upper = model$used_args$upper)
  if(mod2$ll > model$ll) model <- mod2
}
C_hat <- C_GP(model)
# Compute subspace distance
ssd[nit] <- subspace_dist(C_hat, matrix(act_dir, nrow = nvar), r = 1)
}
plot(ssd, type = 'b')

```

C_GP

C matrix closed form expression for a GP.

Description

Computes the integral (uniform measure) over the [0,1] box domain of the outer product of the gradients of a Gaussian process. The corresponding matrix is the C matrix central in the active subspace methodology.

Usage

```
C_GP(model)
```

Arguments

model	homGP or hetGP GP model, see hetGP-package containing, e.g., a vector of thetas, type of covariance ct, an inverse covariance matrix Ki, a design matrix X0, and response vector Z0.
-------	--

Value

a const_C object with elements

- model: GP model provided;
- mat: C matrix estimated;
- Wij: list of W matrices, of size number of variables;
- ct: covariance type (1 for "Gaussian", 2 for "Matern3_2", 3 for "Matern5_2").

References

N. Wycoff, M. Binois, S. Wild (2019+), Sequential Learning of Active Subspaces, preprint.

P. Constantine (2015), Active Subspaces, Philadelphia, PA: SIAM.

Examples

```
#####
### Active subspace of a Gaussian process
#####
library(hetGP); library(lhs)
set.seed(42)

nvar <- 2
n <- 100

# theta gives the subspace direction
f <- function(x, theta, nugget = 1e-3){
  if(is.null(dim(x))) x <- matrix(x, 1)
  xact <- cos(theta) * x[,1] - sin(theta) * x[,2]
  return(hetGP::f1d(xact) + rnorm(n = nrow(x), sd = rep(nugget, nrow(x))))
}

theta_dir <- pi/6
act_dir <- c(cos(theta_dir), -sin(theta_dir))

# Create design of experiments and initial GP model
design <- X <- matrix(signif(maximinLHS(n, nvar), 2), ncol = nvar)
response <- Y <- apply(design, 1, f, theta = theta_dir)
model <- mleHomGP(design, response, known = list(beta0 = 0))

C_hat <- C_GP(model)

# Subspace distance to true subspace:
print(subspace_dist(C_hat, matrix(act_dir, nrow = nvar), r = 1))
plot(design %*% eigen(C_hat$mat)$vectors[,1], response,
     main = "Projection along estimated active direction")
plot(design %*% eigen(C_hat$mat)$vectors[,2], response,
     main = "Projection along estimated inactive direction")
```

C_GP_ci

*CI on Eigenvalues via Monte Carlo/GP***Description**

CI on Eigenvalues via Monte Carlo/GP

Usage

C_GP_ci(model, B = 100)

Arguments

model	A homGP model
B	Monte Carlo iterates

Value

A list with elements ci giving 95

Examples

```
#####
## Example of uncertainty quantification on C estimate
#####
library(hetGP); library(lhs)
set.seed(42)

nvar <- 2
n <- 20
nits <- 20

# theta gives the subspace direction
f <- function(x, theta, nugget = 1e-6){
  if(is.null(dim(x))) x <- matrix(x, 1)
  xact <- cos(theta) * x[,1] - sin(theta) * x[,2]
  return(hetGP::f1d(xact) + rnorm(n = nrow(x), sd = rep(nugget, nrow(x))))
}

theta_dir <- pi/6
act_dir <- c(cos(theta_dir), -sin(theta_dir))

# Create design of experiments and initial GP model
design <- X <- matrix(signif(maximinLHS(n, nvar), 2), ncol = nvar)
response <- Y <- apply(design, 1, f, theta = theta_dir)
model <- mleHomGP(design, response, known = list(beta0 = 0))

res <- C_GP_ci(model)

plot(c(1, 2), log(c(mean(res$eigen_draws[,1]), mean(res$eigen_draws[,2]))),
  ylim = range(log(res$eigen_draws)), ylab = "Eigenvalue", xlab = "Index")
  segments(1, log(res$ci[1,1]), 1, log(res$ci[2,1]))
  segments(2, log(res$ci[1,2]), 2, log(res$ci[2,2]))
```

C_tr

Expected variance of trace of C

Description

Expected variance of trace of C

Usage

C_tr(C, xnew, grad = FALSE)

Arguments

C	A const_C object, the result of a call to C_GP.
xnew	The new design point
grad	If FALSE, calculate variance of trace after update. If TRUE, returns the gradient.

Value

A real number giving the expected variance of the trace of C given the current design.

References

N. Wycoff, M. Binois, S. Wild (2019+), Sequential Learning of Active Subspaces, preprint.

Examples

```
#####
### Variance of trace criterion landscape
#####
library(hetGP)
set.seed(42)
nvar <- 2
n <- 20

# theta gives the subspace direction
f <- function(x, theta = pi/6, nugget = 1e-6){
  if(is.null(dim(x))) x <- matrix(x, 1)
  xact <- cos(theta) * x[,1] - sin(theta) * x[,2]
  return(hetGP::f1d(xact) +
    rnorm(n = nrow(x), sd = rep(nugget, nrow(x))))
}

design <- matrix(signif(runif(nvar*n), 2), ncol = nvar)
response <- apply(design, 1, f)
model <- mleHomGP(design, response, lower = rep(1e-4, nvar),
  upper = rep(0.5,nvar), known = list(g = 1e-4))

C_hat <- C_GP(model)

ngrid <- 101
xgrid <- seq(0, 1,, ngrid)
Xgrid <- as.matrix(expand.grid(xgrid, xgrid))
filled.contour(matrix(f(Xgrid), ngrid))

Ctr_grid <- apply(Xgrid, 1, C_tr, C = C_hat)
filled.contour(matrix(Ctr_grid, ngrid), color.palette = terrain.colors,
  plot.axes = {axis(1); axis(2); points(design, pch = 20)}))
```

C_var	<i>Element-wise Cn+1 variance</i>
-------	-----------------------------------

Description

Element-wise Cn+1 variance

Usage

```
C_var(C, xnew, grad = FALSE)
```

Arguments

C	A const_C object, the result of a call to <code>C_GP</code> .
xnew	The new design point
grad	If FALSE, calculate variance of update. If TRUE, returns the gradient.

Value

A real number giving the expected elementwise variance of C given the current design.

References

N. Wycoff, M. Binois, S. Wild (2019+), Sequential Learning of Active Subspaces, preprint.

Examples

```
#####
### Norm of the variance of C criterion landscape
#####
library(hetGP)
set.seed(42)
nvar <- 2
n <- 20

# theta gives the subspace direction
f <- function(x, theta = pi/6, nugget = 1e-6){
  if(is.null(dim(x))) x <- matrix(x, 1)
  xact <- cos(theta) * x[,1] - sin(theta) * x[,2]
  return(hetGP::f1d(xact)
    + rnorm(n = nrow(x), sd = rep(nugget, nrow(x))))
}

design <- matrix(signif(runif(nvar*n), 2), ncol = nvar)
response <- apply(design, 1, f)
model <- mleHomGP(design, response, lower = rep(1e-4, nvar),
  upper = rep(0.5, nvar), known = list(g = 1e-4))
```

```

C_hat <- C_GP(model)

ngrid <- 51
xgrid <- seq(0, 1,, ngrid)
Xgrid <- as.matrix(expand.grid(xgrid, xgrid))
filled.contour(matrix(f(Xgrid), ngrid))

cvar_crit <- function(C, xnew){
  return(sqrt(sum(C_var(C, xnew)^2)))
}

Cvar_grid <- apply(Xgrid, 1, cvar_crit, C = C_hat)
filled.contour(matrix(Cvar_grid, ngrid), color.palette = terrain.colors,
  plot.axes = {axis(1); axis(2); points(design, pch = 20)})

```

C_var2

Alternative Variance of Update

Description

Defined as $E[(C - E[C])^2]$, where $A^2 = AA$ (not elementwise multiplication).

Usage

```
C_var2(C, xnew, grad = FALSE)
```

Arguments

C	A const_C object, the result of a call to C_GP .
xnew	The new design point
grad	If FALSE, calculate variance of update. If TRUE, returns the gradient.

Value

A real number giving the expected variance of C defined via matrix multiplication given the current design.

References

N. Wycoff, M. Binois, S. Wild (2019+), Sequential Learning of Active Subspaces, preprint.

Examples

```
#####
### Norm of the variance of C criterion landscape
#####
library(hetGP)
set.seed(42)
nvar <- 2
n <- 20

# theta gives the subspace direction
f <- function(x, theta = pi/6, nugget = 1e-6){
  if(is.null(dim(x))) x <- matrix(x, 1)
  xact <- cos(theta) * x[,1] - sin(theta) * x[,2]
  return(hetGP::f1d(xact) + rnorm(n = nrow(x), sd = rep(nugget, nrow(x))))
}

design <- matrix(signif(runif(nvar*n), 2), ncol = nvar)
response <- apply(design, 1, f)
model <- mleHomGP(design, response, lower = rep(1e-4, nvar),
                 upper = rep(0.5, nvar), known = list(g = 1e-4))

C_hat <- C_GP(model)

ngrid <- 51
xgrid <- seq(0, 1, , ngrid)
Xgrid <- as.matrix(expand.grid(xgrid, xgrid))
filled.contour(matrix(f(Xgrid), ngrid))

cvar_crit <- function(C, xnew){
  return(sqrt(sum(C_var(C, xnew)^2)))
}

Cvar_grid <- apply(Xgrid, 1, cvar_crit, C = C_hat)
filled.contour(matrix(Cvar_grid, ngrid), color.palette = terrain.colors,
                 plot.axes = {axis(1); axis(2); points(design, pch = 20)})
```

domain_to_R

Rectangular Domain -> Unbounded Domain

Description

Given an m dimensional function whose inputs live in bounded intervals $[a_1, b_1]$, ..., $[a_m, b_m]$, return a wrapped version of the function whose inputs live in \mathbb{R}^m . Transformed using the logit function.

Usage

```
domain_to_R(f, domain)
```

Arguments

f The function to wrap, should have a single vector-valued input.
 domain A list of real tuples, indicating the original domain of the function.

Value

A function wrapping f.

domain_to_unit *Change a function's inputs to live in [-1, 1]*

Description

Given an m dimensional function whose inputs live in bounded intervals [a1, b1], ..., [am, bm], return a wrapped version of the function whose inputs live in [-1, 1], ..., [-1, 1].

Usage

domain_to_unit(f, domain)

Arguments

f The function to wrap, should have a single vector-valued input.
 domain A list of real tuples, indicating the original domain of the function.

Value

A function wrapping f.

grad_est_subspace *Estimate the Active Subspace of a Cheap Function using Gradients*

Description

Looks between [-1, 1]

Usage

grad_est_subspace(f, r, m, M = NULL, scale = FALSE)

Arguments

f	The function to eval
r	The max dim of the active subspace
m	The dimension of the underlying/embedding space.
M	optional budget of evaluations, default to $2 * r * \log(m)$
scale	Scale all gradients to have norm 1?

Value

A list with sub, the active subspace, sv, the singular values (all m of them), fs, which gives function values, gs, function grads, and X, which gives sampled locations.

logLikHessian	<i>Hessian of the log-likelihood with respect to lengthscales hyperparameters Works for homGP and hetGP models from the hetGP package for now.</i>
---------------	--

Description

Hessian of the log-likelihood with respect to lengthscales hyperparameters Works for homGP and hetGP models from the hetGP package for now.

Usage

```
logLikHessian(model)
```

Arguments

model	homGP model
-------	-------------

Value

A matrix giving the Hessian of the GP loglikelihood.

n11_2_01	<i>f:[-1, 1] -> R Becomes f:[0,1] -> R</i>
----------	--

Description

f:[-1, 1] -> R Becomes f:[0,1] -> R

Usage

n11_2_01(f)

Arguments

f initial function

Value

The same function with domain shifted.

print.const_C	<i>Print const_C objects</i>
---------------	------------------------------

Description

Print const_C objects

Usage

```
## S3 method for class 'const_C'
print(x, ...)
```

Arguments

x A const_C object, the result of a call to C_GP
 ... Additional parameters. Not used.

subspace_dist	<i>Get the distance between subspaces defined as the ranges of A and B</i>
---------------	--

Description

Get the distance between subspaces defined as the ranges of A and B

Usage

```
subspace_dist(A, B, r)
```

Arguments

A	A matrix or const_C object.
B	Another matrix with the same number of rows as A, or const_C object of the same dimension.
r	A scalar integer, the dimension of the subspace to compare (only necessary if either A or B is a const_C object).

Value

A nonnegative scalar giving the cosine of the first principle angle between the two subspaces.

update.const_C	<i>C update with new observations</i>
----------------	---------------------------------------

Description

Update Constantine's C with new point(s) for a GP

Usage

```
## S3 method for class 'const_C'
update(object, Xnew, Znew, ...)
```

Arguments

object	A const_C object, the result of a call to the C_GP function.
Xnew	matrix (one point per row) corresponding to the new designs
Znew	vector of size nrow(Xnew) for the new responses at Xnew
...	not used (for consistency of update method)

Value

The updated const_C object originally provided.

See Also

`C_GP` to generate `const_C` objects from `mleHomGP` objects; `update_C2` for an update using faster expressions.

Examples

```
#####
### Active subspace of a Gaussian process
#####
library(hetGP); library(lhs)
set.seed(42)

nvar <- 2
n <- 100

# theta gives the subspace direction
f <- function(x, theta, nugget = 1e-3){
  if(is.null(dim(x))) x <- matrix(x, 1)
  xact <- cos(theta) * x[,1] - sin(theta) * x[,2]
  return(hetGP::f1d(xact) +
    rnorm(n = nrow(x), sd = rep(nugget, nrow(x))))
}

theta_dir <- pi/6
act_dir <- c(cos(theta_dir), -sin(theta_dir))

# Create design of experiments and initial GP model
design <- X <- matrix(signif(maximinLHS(n, nvar), 2), ncol = nvar)
response <- Y <- apply(design, 1, f, theta = theta_dir)
model <- mleHomGP(design, response, known = list(beta0 = 0))

C_hat <- C_GP(model)

print(C_hat)
print(subspace_dist(C_hat, matrix(act_dir, nrow = nvar), r = 1))

# New designs
Xnew <- matrix(runif(2), 1)
Znew <- f(Xnew, theta_dir)

C_new <- update(C_hat, Xnew, Znew)
print(C_new)
subspace_dist(C_new, matrix(act_dir, nrow = nvar), r = 1)
```

Description

Update Constantine's C, using update formula

Usage

```
update_C2(C, xnew, ynew)
```

Arguments

C	A const_C object, the result of a call to C_GP .
xnew	The new design point
ynew	The new response

Value

Updated C matrix, a const_C object.

References

N. Wycoff, M. Binois, S. Wild (2019+), Sequential Learning of Active Subspaces, preprint.

Index

`activegp`, 2

`C_GP`, 4, 7–9, 15, 16

`C_GP_ci`, 5

`C_tr`, 6

`C_var`, 8

`C_var2`, 9

`domain_to_R`, 10

`domain_to_unit`, 11

`grad_est_subspace`, 11

`logLikHessian`, 12

`mleHomGP`, 15

`n11_2_01`, 13

`print.const_C`, 13

`subspace_dist`, 14

`update.const_C`, 14

`update_C2`, 15, 15