

# lineqGPR\_MaxModAlgorithm\_Monotonicity5D

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## 1 Demo: Gaussian processes under monotonicity constraints

In this notebook, we propose a demo example of the implementation of a Gaussian process (GP) under monotonicity constraints. The model is constructed via the MaxMod algorithm proposed in [1]

[1] F. Bachoc, A. F. López-Lopera, and O. Roustant. *Sequential construction and dimension reduction of Gaussian processes under inequality constraints*. 2020. URL: <https://arxiv.org/abs/2009.04188>.

```
[1]: # loading useful libraries
library("lineqGPR")
require("DiceDesign")
library("plot3D")
library("viridis")

rm(list=ls())
options(warn=-1)
```

Warning message:

"package 'lineqGPR' was built under R version 4.0.4"

Loading required package: broom

Warning message:

"package 'broom' was built under R version 4.0.4"

Loading required package: nloptr

Loading required package: purrr

Loading required package: DiceDesign

Warning message:

"package 'DiceDesign' was built under R version 4.0.4"

Loading required package: viridisLite

```
[2]: # Synthetic data: monotonic function
modatan <- function(x, a) return(atan(a*x))
```

```
targetFun <- function(x, d) {
  y <- 0
  a <- (1-(1:d)/(d+1))*5
  for (k in 1:d)
    y <- y + modatan(x[, k], a[k])
  return(y)
}
```

```
[3]: D <- 5 # number of active + inactive input variables
d <- 2 # number of active input variables

# building DoE in dimension D via Latin hypercube sampling (LHS)
nbtrain <- 20*D # nb of training data
xdesign <- lhsDesign(nbtrain, D, seed = 8)$design
xdesign <- maximinSA_LHS(xdesign)$design
ydesign <- targetFun(xdesign, d)

# building a DoE for assessing the model
ntest <- 80*D # nb of test data for the MaxMod criterion
xtest <- lhsDesign(ntest, D, seed = 8)$design
xtest <- maximinSA_LHS(xtest)$design
```

```
[4]: # initializing a 1D GP model with only two knots
model <- create(class = 'lineqMaxModGP',
               x = rep(0, nbtrain), y = ydesign,
               constrType = c("monotonicity"))
model$localParam$m <- 2
model$uinit <- lapply(1:D, function(x) seq(0, 1, length.out =
  ↪model$localParam$m))
model$varnoise <- var(ydesign)
model$kernParam$nugget <- 1e-5
```

```
[5]: # updating the model according to the MaxMod algorithm
model <- MaxMod(model,
               xdesign,
               xtest,
               D = D,
               tol = 1e-5,
               max_iter = 10*model$d,
               reward_new_knot = 1e-6,
               reward_new_dim = 1e-9,
               print_iter = TRUE,
               nClusters = 10,
               save_history = TRUE)

message("\nNumber of active dimensions: ", d)
message("Number of actived dimensions via MaxMod: ", model$d, "\n")
```

	dim 1	dim 2	dim 3	dim 4	dim 5
MaxMod criterion	1.224175	1.218699	1.179208	1.177648	1.177618
knot's position	NaN	NaN	NaN	NaN	NaN
decision	1.000000	0.000000	0.000000	0.000000	0.000000

Iter 1 - dimension 1 added as d = 1 (MaxMod criterion = 1.22417501911793)

  

	dim 1	dim 2	dim 3	dim 4	dim 5
MaxMod criterion	0.01929934	0.04792809	0.0001420925	0.0005257585	0.0003219
knot's position	0.38289803	NaN	NaN	NaN	NaN
decision	0.00000000	1.00000000	0.0000000000	0.0000000000	0.00000000

Iter 2 - dimension 2 added as d = 2 (MaxMod criterion = 0.0479280915949658)

  

	dim 1	dim 2	dim 3	dim 4	dim 5
MaxMod criterion	0.006794792	0.002083112	0.0001107679	7.457895e-05	2.856565e-05
knot's position	0.387948087	0.401963016	NaN	NaN	NaN
decision	1.000000000	0.000000000	0.0000000000	0.000000e+00	0.000000e+00

Iter 3 - New knot added: d = 1 (MaxMod criterion = 0.00679479216792167)

  

	dim 1	dim 2	dim 3	dim 4
MaxMod criterion	5.236616e-05	0.001063286	7.126979e-05	2.696419e-05
knot's position	6.873642e-01	0.459725552	NaN	NaN
decision	0.000000e+00	1.000000000	0.000000e+00	0.000000e+00

  

	dim 5
MaxMod criterion	1.594172e-05
knot's position	NaN
decision	0.000000e+00

Iter 4 - New knot added: d = 2 (MaxMod criterion = 0.00106328550109741)

  

	dim 1	dim 2	dim 3	dim 4
MaxMod criterion	4.742941e-05	3.591556e-05	2.637898e-05	5.199535e-06
knot's position	7.513662e-01	6.762894e-01	NaN	NaN
decision	1.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00

  

	dim 5
MaxMod criterion	9.179307e-06
knot's position	NaN
decision	0.000000e+00

Iter 5 - New knot added: d = 1 (MaxMod criterion = 4.74294056228348e-05)

  

	dim 1	dim 2	dim 3	dim 4
MaxMod criterion	0.0002100842	2.853189e-05	1.534378e-05	4.131272e-06
knot's position	0.2132356442	6.698371e-01	NaN	NaN
decision	1.0000000000	0.000000e+00	0.000000e+00	0.000000e+00

  

	dim 5
--	-------

MaxMod criterion 8.518938e-06  
knot's position NaN  
decision 0.000000e+00

Iter 6 - New knot added: d = 1 (MaxMod criterion = 0.000210084175922863)

	dim 1	dim 2	dim 3	dim 4
MaxMod criterion	1.124038e-05	1.794553e-05	7.648012e-06	1.185838e-06
knot's position	6.009299e-01	7.039008e-01	NaN	NaN
decision	0.000000e+00	1.000000e+00	0.000000e+00	0.000000e+00

dim 5  
MaxMod criterion 1.723864e-06  
knot's position NaN  
decision 0.000000e+00

Iter 7 - New knot added: d = 2 (MaxMod criterion = 1.79455339766526e-05)

	dim 1	dim 2	dim 3	dim 4
MaxMod criterion	8.448796e-06	3.235447e-05	6.062107e-06	1.673104e-06
knot's position	5.388241e-01	1.285831e-01	NaN	NaN
decision	0.000000e+00	1.000000e+00	0.000000e+00	0.000000e+00

dim 5  
MaxMod criterion 1.858297e-06  
knot's position NaN  
decision 0.000000e+00

Iter 8 - New knot added: d = 2 (MaxMod criterion = 3.23544665059667e-05)

	dim 1	dim 2	dim 3	dim 4
MaxMod criterion	1.614464e-05	2.128111e-05	5.648488e-06	2.968942e-06
knot's position	6.272510e-01	2.056282e-01	NaN	NaN
decision	0.000000e+00	1.000000e+00	0.000000e+00	0.000000e+00

dim 5  
MaxMod criterion 8.261117e-06  
knot's position NaN  
decision 0.000000e+00

Iter 9 - New knot added: d = 2 (MaxMod criterion = 2.12811139487102e-05)

	dim 1	dim 2	dim 3	dim 4
MaxMod criterion	1.648198e-05	2.127745e-06	5.070316e-06	2.849696e-06
knot's position	6.506193e-01	3.496223e-01	NaN	NaN
decision	1.000000e+00	0.000000e+00	0.000000e+00	0.000000e+00

dim 5  
MaxMod criterion 7.199773e-06  
knot's position NaN  
decision 0.000000e+00

Iter 10 - New knot added:  $d = 1$  (MaxMod criterion = 1.64819797380224e-05)

Run out of budget

Number of active dimensions: 2

Number of actived dimensions via MaxMod: 2

```
[6]: # evaluating the model using an equispaced grid of points
ntest <- 10
xtestGrid <- as.matrix(expand.grid(seq(0, 1, length = ntest), seq(0, 1, length =
  ↳ ntest)))
ytestGrid <- targetFun(xtestGrid, d)
pred <- predict(model, xtestGrid)

[7]: # plotting the MAP estimate
colormap <- rev(viridis(1e2))
options(repr.plot.width = 15, repr.plot.height = 6)
par(mfrow = c(1,2))
p <- persp3D(x = seq(0, 1, length = ntest), y = seq(0, 1, length = ntest),
  z = matrix(pred$Phi.test %*% pred$xi.map, nrow = ntest),
  xlab = "x2", ylab = "x1", zlab = "y(x1,x2)",
  main = "target function",
  phi = 20, theta = -30, col = colormap,
  contour = TRUE, colkey=FALSE, lwd = 4)
points3D(x = model$x[, 1], y = model$x[, 2], z = ydesign,
  col = 'black', pch = 19, add=TRUE)
u <- expand.grid(model$u[[1]], model$u[[2]])
pred_Knots <- predict(model, as.matrix(u))
points(trans3D(x = u[, 1], y = u[, 2], z = pred_Knots$Phi.test %*%
  ↳ pred_Knots$xi.map, pmat = p),
  col = 'brown', pch = 4, lwd = 4)

diff = ytestGrid - pred$Phi.test %*% pred$xi.map
image2D(abs(matrix(diff, nrow = ntest)), col = rev(colormap),
  main = "absolute error", xlab = "x2", ylab = "x1")
points2D(model$x[, 1], model$x[, 2], add = TRUE, pch = 19, col = 'black')
points2D(u[, 1], u[, 2], add = TRUE, pch = 4, lwd = 4, col = 'brown')
```

