The Revised Sequential Parameter Optimization Toolbox

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Sequential Parameter Optimization: Overview

- Developed: Bartz-Beielstein et al. (2005)
- Core purpose:
  - Derive understanding of problem, parameters
  - Reduce load of costly target functions
  - Statistically sound comparisons
- Combines approaches from different fields
  - Design of Experiment
  - Statistics
  - Optimization algorithms
- Areas of application
  - Algorithm tuning
  - Engineering design
  - And many more (Bartz-Beielstein, 2010)
- R-package maintained by SPOTSeven research group
Sequential Parameter Optimization: Concept

Create initial design → Evaluate design → Goal Reached? → No → Build a surrogate model → Optimize surrogate model → Update design

Goal Reached? → Yes → Analyse and report results
unknown target function
Create initial design → Evaluate design

Goal Reached?

Yes →

No →

Build a surrogate model → Optimize surrogate model → Update design

Analyse and report results

initial design
Create initial design  
Evaluate design  
Goal Reached?  
No  
Build a surrogate model  
Optimize surrogate model  
Update design  
Yes  
Analyse and report results

f(x)

evaluate initial design

analyze and report results

S. Krey (TH Köln)
Create initial design → Evaluate design → Goal Reached?
Yes → Build a surrogate model → Optimize surrogate model → Update design
No → Analyse and report results

\( f(x) \) → build surrogate model

\( x \)
optimize surrogate model

Create initial design → Evaluate design → Goal Reached?

Yes → Analyse and report results

No → Build a surrogate model → Optimize surrogate model → Update design

$f(x)$

optimize surrogate model

S. Krey (TH Köln)
Create initial design → Evaluate design → Goal Reached? → No → Build a surrogate model → Optimize surrogate model → Update design → Analyse and report results

$\text{evaluate}$

$f(x)$

$x$
Create initial design → Evaluate design → Goal Reached?
  No → Build a surrogate model → Optimize surrogate model → Update design
  Yes → Analyse and report results

\[ f(x) \]

build surrogate model

\[ \text{goal reached?} \]

\[ \text{update design} \]
Create initial design → Evaluate design → Build surrogate model → Optimize surrogate model → Update design

Goal Reached?

Yes → Analyse and report results

No → Create initial design

$f(x)$

optimize surrogate model
Create initial design → Evaluate design → Goal Reached?

Yes → Analyse and report results

No → Build a surrogate model → Optimize surrogate model → Update design

Goal Reached? → Yes

f(x) → x

evaluate

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Create initial design → Evaluate design → Goal Reached?

Yes → Build a surrogate model → Optimize surrogate model → Update design

No → Analyse and report results

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$f(x)$

build surrogate model
Create initial design → Evaluate design → Analyse and report results → Optimize surrogate model → Update design

Goal Reached?
Yes → Optimize surrogate model
No → Build a surrogate model

$f(x)$

optimize surrogate model
Create initial design → Evaluate design → Goal Reached? Yes → Analyse and report results → f(x) success

Goal Reached? No → Build a surrogate model → Optimize surrogate model → Update design
Aims of the revised SPOT package

- High prediction quality
- Stable numerics
- Fast
- Modular structure for good extensibility
- Standardized objects and user interfaces
- Easy comprehensible code
- Good usability
What is new?

- No text files for configuration and data exchange anymore
- Everything implemented in R
- Object-oriented data structures as input and output for the individual functions
- Consistent with core R functionality
- Standardized and modular structure of the functions form a harmonized and easy understandable user interface
- Kriging with categorical inputs
- Stacking of different models for better prediction performance
  Bartz-Beielstein and Zaefferer (2017)
Create initial design

designLHD(x = NULL, lower, upper, control = list())

- **Arguments**
  - **x**: optional matrix of fixed user defined design points
  - **lower/upper**: vectors with boundaries for the design variables
  - **control**: list with the following controls:
    - **size**: number of design points
    - **retries**: number of retries during design creation
    - **types**: vector with the data type for each design parameter
    - **replicates**: integer for replications of each design point
  
- Returns matrix with design points (rows) for each variable (columns)
Model building

Different models can be chosen

- Linear models
- Kriging / Gaussian process regression
- Random Forest
- ...

buildKriging(x, y, control = list())

Arguments

- x: design matrix (sample locations)
- y: vector of observations at x
- control: list with the options for the model building procedure

Returns an object of class kriging, basically a list, with the options and found parameters for the model which has to be passed to the predictor function
Optimization

optimLBFGSB(x = NULL, fun, lower, upper, control = list(), ...)

- Wrapper function for optim with method = "L-BFGS-B"
- Arguments
  - **x**: optional matrix of data-points, only first row used as start-point
  - **fun**: objective function, which receives a matrix x and returns observations y
  - **lower/upper**: boundary of the search space
  - **control**: list of control parameters, passed to optim
  - **funEvals**: number of function evaluations allowed
  - ...: passed to fun
- Returns list with best solution (xbest, ybest), number of function evaluations (count) and messages from the optimizer
Why SPOT instead of package . . .

A lot of packages provide methods for model based optimization, Kriging, etc. For example mlrMBO, diceKriging, diceOptim, mleGP, . . .

- easy usage
- own Kriging implementation for stable numerics (based on Matlab code from Forrester et al. (2008))
- fast
- good and easy extensibility
- well proven methods for good results in real world problems
Cyclone optimization

Front View

Top View

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funCyclone(c(1260,2500)) #[1] 1626.194527 -0.886269
## create vectorized target funcion for the first objective only
tfunvecF1 <- function(x){apply(x,1,funCyclone)[2,]}
fixed <- matrix(c(1260,2500,1000,2000),2,2,byrow=TRUE)
lower <- c(1000,2000)
upper <- c(2000,3000)
## optimize with spot
res <- spot(x = designLHD(x = fixed, lower = lower, upper = upper, control = list(size=4)),
            fun = tfunvecF1,
            lower = lower,
            upper = upper,
            control = list(modelControl = list(target="ei"),
                            model = buildKriging,
                            optimizer = optimLBFGSB,
                            plots=TRUE))
## best found solution ...
res$xbest #[1,] 2000 2861.775
## ... and its objective function value
res$ybest #[1,] -0.95085
Cyclone optimization

A more complex cyclone optimization, building a stacking ensemble of models from lab experiments, CFD simulations and analytical models can be found in Bartz-Beielstein et al. (2016).

The necessary datasets and the source code for this optimization is available here: http://www.gm.fh-koeln.de/~bartz/Bart16e.d/
Stacking example

require(SPOT); require(CEGO)

train <- dataGasSensor[dataGasSensor[,11]==1,1:10]
test <- dataGasSensor[dataGasSensor[,11]==2,1:10]

#define an optimizer:
optimizer <- function(x,fun,lower,upper,control,...){
  CEGO::optimInterface(x, fun, lower, upper,
        control=list(method="NLOPT_GN_DIRECT_L", funEvals=10,
                     reltol=1e-6, restarts=2), ...)
}

fitStack <- buildEnsembleStack(
  data.matrix(train[,c("Y","X7","Sensor","Batch")]),
  data.matrix(train$X1),
  control=list(modelL0Control=list(list(), list(),
                               list(algTheta=optimizer,reinterpolate=FALSE)
                           )
  )
)
predtest <- predict(fitStack,
  data.matrix(test[,c("Y","X7","Sensor","Batch")]))$y
mse <- mean(abs(predtest - data.matrix(test$X1))^2) # [1] 0.2627715
Stacking example
Summary and Outlook

- SPOT 2 provides a good base for real world optimization problems
- Interfaces and object structures are stable and allow easy extensions
- Reporting functions are still missing (current work in progress)
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Thank you for your attention!
References


