Sequential Parameter Optimization for Symbolic Regression

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SPOT SEVEN
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Agenda

R: Programming Language for Statistics

- R is "GNU S", a freely available language and environment for statistical computing and graphics.
- R provides a wide variety of statistical and graphical techniques:
  - linear and nonlinear modelling,
  - statistical tests,
  - time series analysis,
  - classification,
  - clustering, etc.
- Useful platform for GP, providing:
  - flexible interactive environment
  - fast expression maniplutaion and evaluation
  - powerful visualization tools
  - tools for parallel computing
- See R project homepage `http://cran.r-project.org/` for further information.

RGP Overview
General Features

- modular GP implementation in R
  - *simplicity beats complexity*
  - *convention over configuration*
- large feature set
  - multiple search heuristics (Pareto GP, TinyGP, ...)
  - multiple representations (tree GP and linear GP)
  - multiple sets of variation operators
  - support for strongly-typed GP
  - $\hookrightarrow$ complex parameterization
- performance-critical functions *also* implemented in C
- comprehensive documentation
- Freely available (GPL-2) on CRAN: `install.packages("rgp")`
- See RGP project homepage `http://rsymbolic.org/` for details and "bleeding edge releases".

GP Search Heuristics

- concrete search strategy employed by a GP system
- independent of the concrete GP search space

$\hookrightarrow$ decouple the search heuristic from the search space

- GP search heuristic components:
  - selection strategy
  - variation pipeline (order of variation operator application)
  - diversity preservation
- GP system components independent of the search heuristic:
  - GP individual representation
  - GP individual initialization and variation (mutation and crossover)
  - GP individual evaluation
- examples of GP search heuristics:
  - classical single-objective steady-state EAs with tournament selection
  - modern multi-objective steady-state heuristics

TinyGP

- popular small GP implementation mainly used in teaching
- steady-state single-objective search heuristic with tournament selection
- no direct means of diversity preservation
- included as a reference with well-known performance characteristics

Table : Parameters of the TinyGP search heuristic.

	Variable (Symbol)	*Domain*	*Default*
Population Size	`mu` (μ)	$\mathbb{N}$	300
Tournament Size	`tournamentSize` ($s_{\text{tournament}}$)	$\mathbb{N}$	2
Recombination Probability	`recombinationProbability` ($p_{\mathtt{rec}}$)	$[0, 1]$	0.9

Generational Multi-Objective GP (GMOGP)

- based on the well-known multi-objective generational $(\mu + \lambda)$ EA NSGAII
- coarsely scalable complexity through optional selection criteria: individual age, individual complexity
- diversity preservation through age-layering
- included as search heuristic with scalable complexity

Table : Parameters of the GMOGP search heuristic.

	Variable (Symbol)	*Domain*	*Default*
Population Size	`mu` (μ)	$\mathbb{N}$	300
Children per Generation	`lambda` (λ)	$\mathbb{N}$	20
New Individuals per Generation	`nu` (ν)	$\mathbb{N}_0$	1
Enable Complexity Criterion	`complexityCriterion`	$\mathbb{B}$	`true`
Enable Age Criterion	`ageCriterion`	$\mathbb{B}$	`true`
Recombination Probability	`recombinationProbability` ($p_{\mathtt{rec}}$)	$[0, 1]$	0.1

Experiment Setup

- *Research goal:* Quantify influence of RGP search heuristic parameters on algorithm performance (single algorithm, single problem).

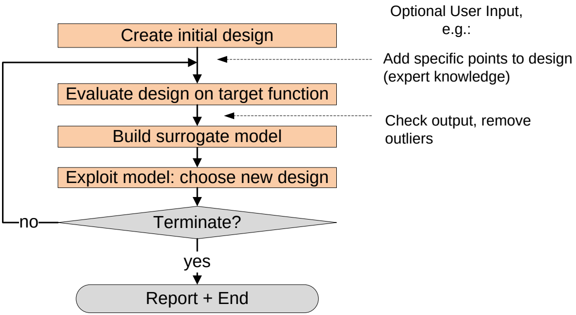
Table : RGP parameters independent of the search heuristic.

Problem	Symbolic Regression of $f(x) := \sin(x) + \cos(2 \cdot x)$
Fitness Cases	200 equidistant samples in $[0, 4 \cdot \pi]$
Error Measure	sample RMSE
Function Set	$\{+, -, \cdot, \div\}$
Input Variable Set	$\{x\}$
Constant Set	uniform random constants in $[-1, 1]$
Individual Size Limit	64
Mutation Operator Set	{ insert/delete subtree, change function/constant }
Crossover Operator Set	{ random subtree crossover }
Time Budget per GP Run	5 minutes
Initial Experiment Design Size	10
Number of Sequential GP Runs	100

SPOT Introduction

Sequential Parameter Optimization [1] Toolbox (SPOT[1])

- Based on statistical methods and Design of Experiment



[1]SPOT and all other used R packages can be retrieved from the CRAN homepage, i.e. `http://cran.r-project.org`.

SPOT Setup

Table : Parameters influencing SPOT performance

Initial Design Size	10
Initial Design Repeats	2
Maximum Repeats	5
Budget (GP-Runs)	100
Old Best Size	3
New Design Size	1
Budget Allocation	Linearly increasing
Surrogate Model	Kriging Model
Surrogate Optimization Method	CMA-ES
Surrogate Optimization Budget	1000

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Interfacing RGP and SPOT I

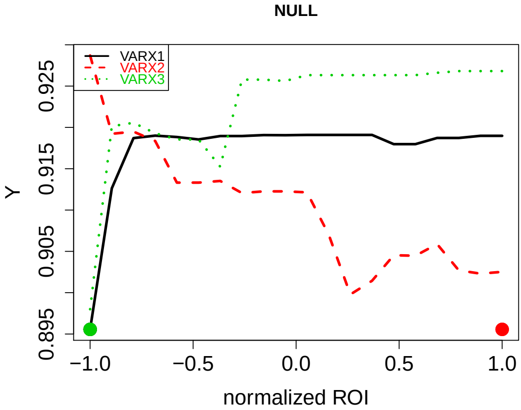
```
> spotRgpTargetFunction <- function(x, time = 120) {
+   populationSize <- x[1]
+   tournamentSizePercentage <- x[2]
+   crossoverProbability <- x[3]
+
+   ## [...]  ## repair parameters as necessary
+
+   ## [...]  ## define problem data, to be solved by symb. regress.
+
+   ## [...]  ## run symbolic regression with parameters
+
+   ## [...]  ## calculate RMSE (fitness) of best individual in population
+
+   return (bestFitness)
+ }
```

Configuring and starting SPOT

```
> conf <- list(alg.func = spotRgpTargetFunction,
+     alg.roi = spotROI(lower  = c(10,   0.0,     0.0),
+                       upper  = c(1000, 1.0,     1.0),
+                       type   = c("INT", "FLOAT", "FLOAT")),
+     alg.seed = 1,
+     spot.seed = 0,
+     seq.predictionModel.func = "spotPredictForrester",
+     seq.predictionOpt.func = "spotPredictOptMulti",
+     seq.predictionOpt.budget = 1000,
+     seq.predictionOpt.method = "cmaes",
+     io.verbosity = 3,
+     report.interactive = TRUE,
+     spot.ocba = FALSE, # no variance at some points causes OCBA to crash
+     init.design.size = 10,
+     init.design.repeats = 2,
+     seq.design.oldBest.size = 3,
+     seq.design.size = 1000,
+     seq.design.new.size = 1,
+     seq.design.maxRepeats = 5,
+     auto.loop.nevals = 100)
> time <- 600 # set per RGP run time budget (in seconds), default is 120
> res <- spot(spotConfig = conf, time = time)
```

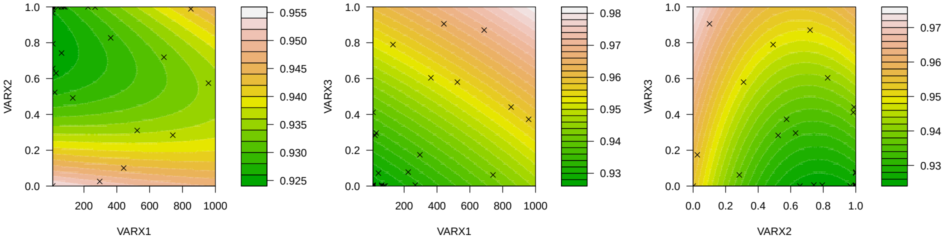
Results of the automated SPOT run

```
> spot(spotConfig=append(
+  list(report.func="spotReportSens"),
+  res),spotTask="rep")
```

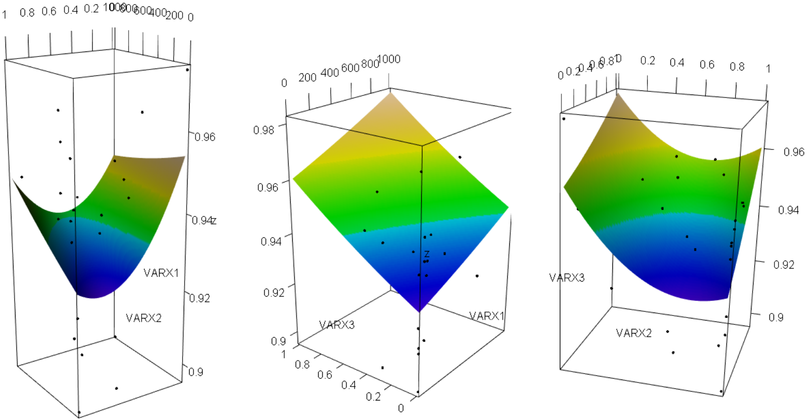


VARX1 (pop. size) VARX2 (tournament size %) VARX3 (crossover prob.)

```
> spot(spotConfig=append(
+  list(report.func="spotReportContour",report.observations.all=T),
+  res),spotTask="rep")
```



```
> spot(spotConfig=append(
+  list(report.func="spotReport3d"),
+  res),spotTask="rep")
```



Factor Variables

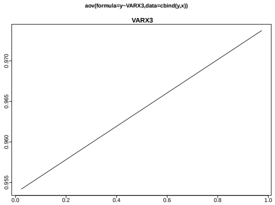
- Categorical Variables
  - Enable Complexity Criterion
  - Enable Age Criterion
- Options
  - Special treatment: Mapping to $\mathbb{R}$ not adequate
  - Analyze each factor setting separately: Many extra runs
  - Random forests
  - Use linear model with dummy variables

Linear Models with Factors

- Initial design: 20 design points $\times$ 2 repeats = 40 GP runs
- 6 variables, 2 factors
- Linear model shows VARX3 (crossover prob.) has significant effect
- Refinement of the automated analysis:
  - Perform stepwise model selection by AIC

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
VARX3	1.000000	0.001389	0.001389	13.577399	0.000711
Residuals	38.000000	0.003887	0.000102		

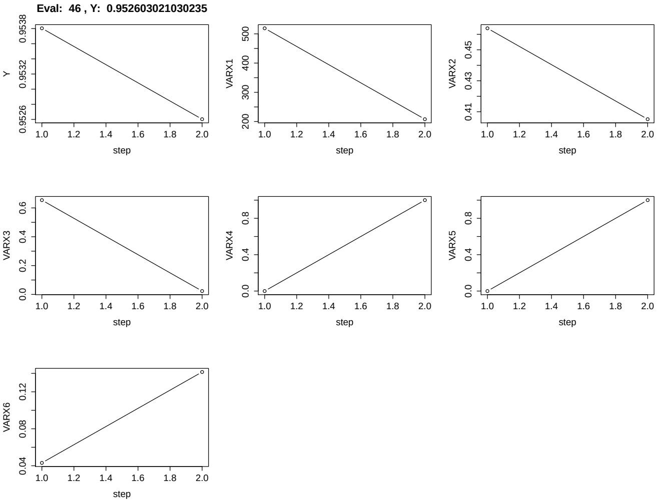
Linear Models: Screening, Model Selection



- Starting 6 additional GP runs to refine the model: 3 old models, 1 new with three repeats

VARX1	VARX2	VARX3	VARX4	VARX5	VARX6	CONFIG	REPEATS	STEP	SEED
519	0.46		0.65	0	0		0.04	2	1
208	0.40		0.02	1	1		0.14	9	1
108	0.26		0.49	0	0		0.96	4	1
75	0.24		0.00	0	0		0.37	21	3

Linear Models: Regression and Dummy Variables



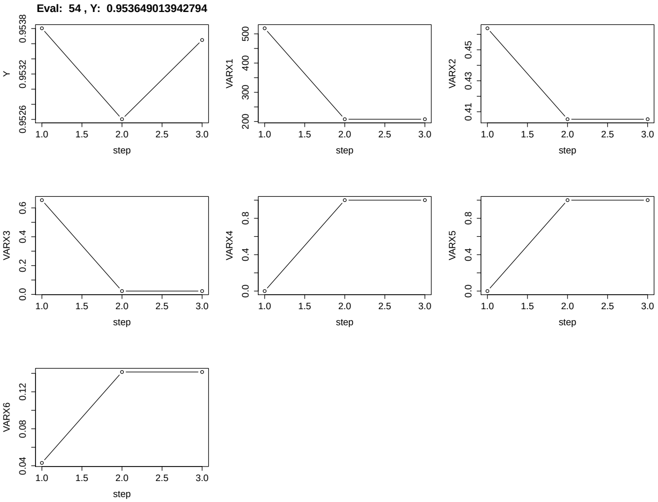
- SPOT search path at step 2

Linear Models: Regression Analysis

- Second step shows similar results.
- Suggested design points after step 2

VARX1	VARX2	VARX3	VARX4	VARX5	VARX6	CONFIG	REPEATS	STEP	SEED
208	0.40	0.02	1	1	0.14	9	1	2	4
108	0.26	0.49	0	0	0.96	4	1	2	4
555	0.54	0.50	1	0	0.91	15	2	2	3
464	0.46	0.00	0	1	0.29	22	4	2	1

Linear Models: Regression and Dummy Variables



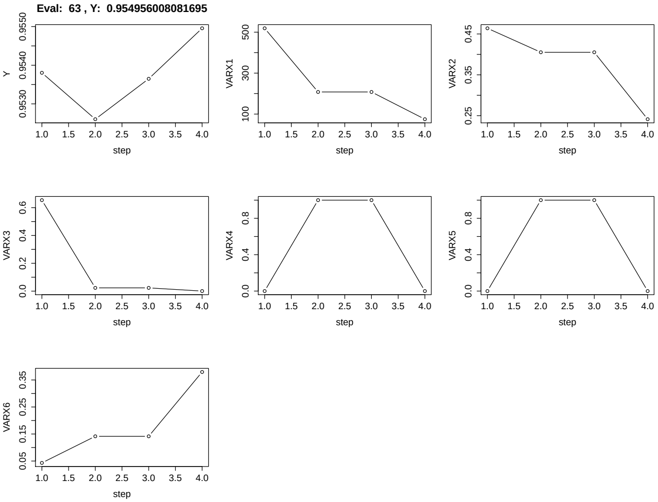
- SPOT search path at step 3

Linear Models: Regression Analysis

- Second step shows similar results.

```
VARX1 VARX2 VARX3 VARX4 VARX5 VARX6 CONFIG REPEATS STEP SEED
208 0.40 0.02 1 1 0.14 9 1  3 5
108 0.26 0.49 0 0 0.96 4 1  3 5
75 0.24 0.00 0 0 0.37 21 2  3 4
352 0.60 0.00 1 1 0.99 23 5  3 1
```

Linear Models: Regression and Dummy Variables



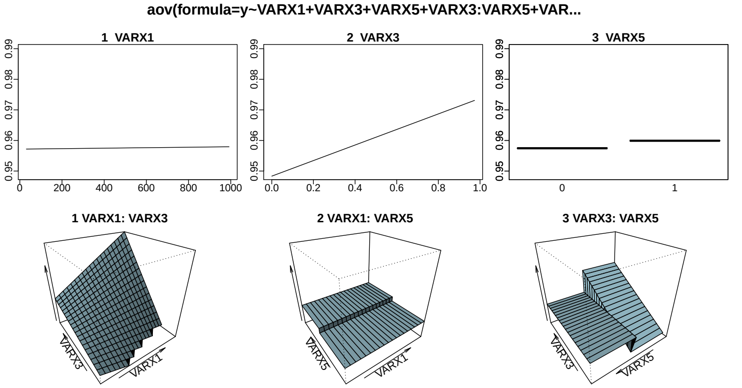
- SPOT search path at step 4

Linear Models with Factors

- Refinement of the automated analysis:
    - Perform stepwise model selection by AIC

	Df	Sum Sq	Mean Sq	F value	Pr(>F)
VARX1	1.000000	0.000588	0.000588	9.403483	0.003309
VARX3	1.000000	0.001004	0.001004	16.056302	0.000180
VARX5	1.000000	0.000048	0.000048	0.765542	0.385272
VARX3:VARX5	1.000000	0.000290	0.000290	4.640992	0.035457
VARX1:VARX3	1.000000	0.000550	0.000550	8.790953	0.004414
Residuals	57.000000	0.003564	0.000063		

Linear Models: Regression and Dummy Variables



- VARX1 + VARX3 + VARX5 + VARX3:VARX5 + VARX1:VARX3
- Interactions between x1 and x5 and between x3 and x5

Summary: Regression Analysis

- Categorical parameters can be easily integrated into the SPOT tuning framework
- More complex models (MARS, GLM) can be used as well, however: Occam's razor
- Crossover prob. has significant impact, should be low
- Children per generation and age criterion: no effect
- Interactions
- Further steps: nested designs for complicated settings

Acknowledgments

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[1] Thomas Bartz-Beielstein, Konstantinos E. Parsopoulos, and Michael N. Vrahatis.
Design and analysis of optimization algorithms using computational statistics.
Applied Numerical Analysis and Computational Mathematics (ANACM), 1(2):413–433, 2004.