Research Topics in Sequential Parameter Optimization

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Optimization via Simulation

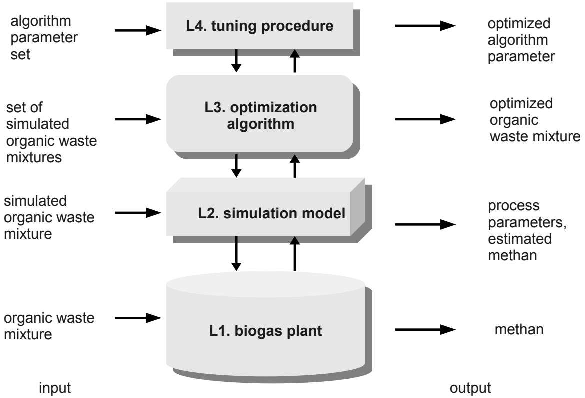
(L1) The real-world system, e.g., a biogas plant

(L2) The related simulation model. The objective function f is defined at this layer. In optimization via simulation, problem parameters are defined at this layer

(L3) The optimization algorithm A. It requires the specification of algorithm parameters, say $\vec{p}^i \in \vec{P}$, where $\vec{P}$ denotes the set of parameter vectors

(L4) The experiments and the tuning procedure

Optimization via Simulation



Sequential Parameter Optimization

- Sequential approach: most powerful optimization technique
- SPOT package can be downloaded from the comprehensive R archive network at `http://CRAN.R-project.org/package=SPOT`
- SPOT is one possible implementation of the *sequential parameter optimization* (SPO) framework introduced in [1]
  - Several implementations developed world wide (SPOT+)
- For a detailed documentation of the functions from the SPOT package, the reader is referred to the package help manuals

Initial Problem Statement

- Developmented started in 2001 at TU Dortmund
- Performance of modern search heuristics such as *evolution strategies* (ES), *differential evolution* (DE), or *simulated annealing* (SANN) relies crucially on their parameterizations—or, statistically speaking, on their factor settings
- *Algorithm design*: factors that influence the behavior (performance) of an algorithm, e.g., population size in ES
- *Problem design*: factors from the optimization (simulation) problem, search space dimension

Tuning

- Interesting goal of SPO: to detect the importance of certain parts (subroutines such as recombination in ES) by systematically varying the factor settings of the algorithm design
- This goal related to improving the algorithm's *efficiency*
- Will be referred to in the following as *algorithm tuning*
- The experimenter is seeking for an improved parameter setting for one problem instance

Robustness

- Varying problem instances, e.g., search space dimensions or starting points of the algorithm, are associated with *effectivity* or the algorithm's robustness
- Experimenter is interested in one parameter setting of the algorithm with which the algorithm performs sufficiently good on several problem instances
- GECCO Tutorial provides an overview, preprint can be downloaded from `http://www.gm.fh-koeln.de/~bartz/Papers.d/Bart12f.pdf`

SPO and DoE

- SPO may lead to a better understanding of the algorithm
- SPO combines several techniques from classical and modern statistics, namely *design of experiments* (DoE) and *design and analysis of computer experiments* (DACE) [1]
- Basic ideas from SPO rely heavily on Kleijnen's work on statistical techniques in simulation [7, 8]
- Book "Experimental methods for the analysis of optimization algorithms" `http://www.springer.com/978-3-642-02537-2` devoted to recent developments in the field of experimental research [3]

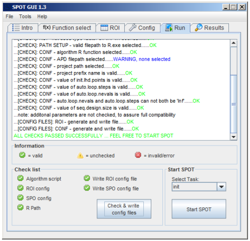
Sequential Parameter Optimization SPO

Use statistical techniques and methods from design of experiment to solve optimization problems.

1. Take initial samples from design space and evaluate on target function/algorithm
2. Build surrogate model (Linear, Tree-based, Kriging, ...) based on known evaluations
3. Determine promising new solutions with model
4. Evaluate new solutions
5. If termination criterion not reached: go to **2.**
6. Summarize Results / Create Report

SPO Toolbox (SPOT)

- Currently maintained and developed as an R-Package
- Interfaces to several other R-packages
- Provides Demos and Documentation
- Graphical User Interface
- Alternative version is available for matlab



SPOT: Installation, Help, Demos

- Install from CRAN:

```
> install.packages("SPOT")
```

- Load package to Workspace:

```
> require("SPOT")
```

- Get help on some spot functions

```
> ?spot
> ?spotOptim
```

- Get a list of SPOT demos

```
> demo(package="SPOT")
```

- Run a SPOT demo

```
> demo("spotDemo18ForresterOptim",ask=F)
```

- Start the GUI

```
> spotGui()
```

Applications: Algorithms Tuned by SPOT

- Several types of evolution strategies
- Time series prediction and anomaly detection
- Classification
- Symbolic Regression
- Simulated Annealing
- For more applications see [2]

Simulated Annealing SANN

- Randomized optimization algorithm
- Two parameters: 1) starting temperature TEMP 2) number of function evaluations at each temperature TMAX

```
> fn <- function (x) {
+  x1 <- x[1] ;  x2 <- x[2]
+  y <- (x2 - 5.1/(4 * pi^2) * (x1^2) + 5/pi * x1 - 6)^2 +
+   10 * (1 - 1/(8 * pi)) * cos(x1) + 10
+  return(y)
+ }
> temp=10; tmax=10
> result<-optim(par=c(-2,3),fn,method="SANN", control = list(temp=temp, tmax=tm
> result$value
```

```
[1] 0.3981833
```

```
> result$par
```

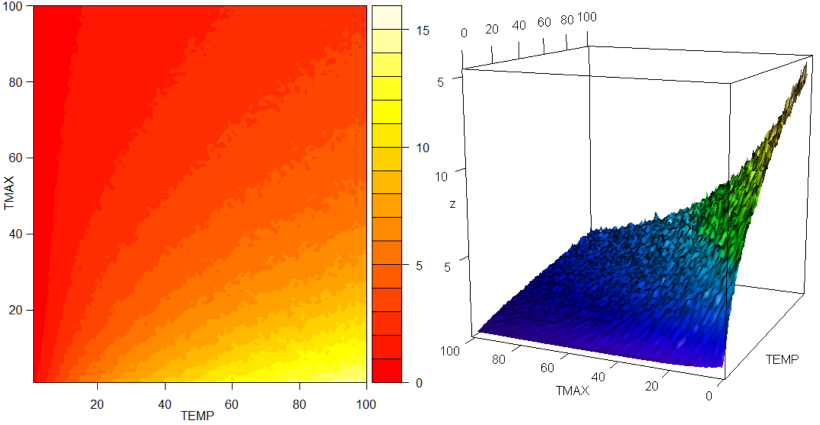
```
[1] -3.144066 12.264619
```

SANN Sweep

- Since this is a simple test problem: Complete sweep
- Understand underlying fitness shape
- 1000 repeats for each setting (takes rather long)

```
> target <- function(x,y,x0,fn,maxit){
+  zz<-matrix(0,length(x))
+  repeats=1000
+  for(i in 1:repeats){
+  set.seed(i)
+  zz =zz + apply(cbind(x,y),1,testalgorithm,x0=x0,fn=fn,maxit=maxit)
+  }
+  return(zz/repeats)
+ }
> x <- seq(1, 100, length.out = 100)
> y <- x
> z <- outer(x, y, target,x0=x0,fn=fn,maxit=maxit)
> filled.contour(x, y, z, color.palette=heat.colors,xlab="temp",ylab="tmax")
> pal <- topo.colors(100)
> require(rgl)
> persp3d(x,y,z,col=pal[cut(z,100)],xlab="TEMP",ylab="TMAX")
```

Plots from Sweep



Tuning SANN in the SPOT Framework: Problem Definition

- Target function: Branin-Function (2-D function with three global minima)

```
> require(SPOT)
> fn <- spotBraninFunction #test function to be optimized by SANN
> x0 <- c(-2,3) #starting point that SANN uses when optimizing Branin
> maxit <- 100 #number of evaluations of Branin allowed for SANN
> testalgorithm <- function(pars,x0,fn,maxit){
+  temp<-pars[1]
+  tmax<-pars[2]
+  y <- optim(x0, fn, method="SANN",
+  control=list(maxit=maxit,
+  temp=temp, tmax=tmax))
+  return(y$value)
+ }
```

Tuning SANN: Configure SPOT

- ROI: Region of interest, in which parameters are tuned
- Surrogate: Kriging based on Forrester et. al. [6]
- Settings are minimalistic (uses a lot of default values)

```
> roi<-spotROI(c(1,1),c(100,100),type=c("INT","INT"))
> config<-list(alg.func=testalgorithm,
+  alg.roi=roi,
+  init.design.size=20,
+  seq.predictionModel.func="spotPredictForrester",
+  seq.predictionOpt.func="spotPredictOptMulti",
+  seq.predictionOpt.method="cmaes",
+  seq.predictionOpt.budget=1000,
+  report.func="spotReportSens",
+  spot.fileMode=T,
+  io.verbosity=3,
+  auto.loop.nevals=100)
```

Tuning SANN: Run SPOT Demo

- Pass configuration to SPOT
- Pass additional parameters to SPOT, needed by target function

```
> # Warning: run takes several minutes
> # (execute from the script sannDemo2012Rome.R)
> # setwd("C:/Users/bartz/Documents/workspace/SvnDdmo.d/trunk/DdmoSlides.d
> res<-spot(spotConfig=config,x0=x0,fn=fn,maxit=maxit)
```

Tuning SANN: Run SPOT

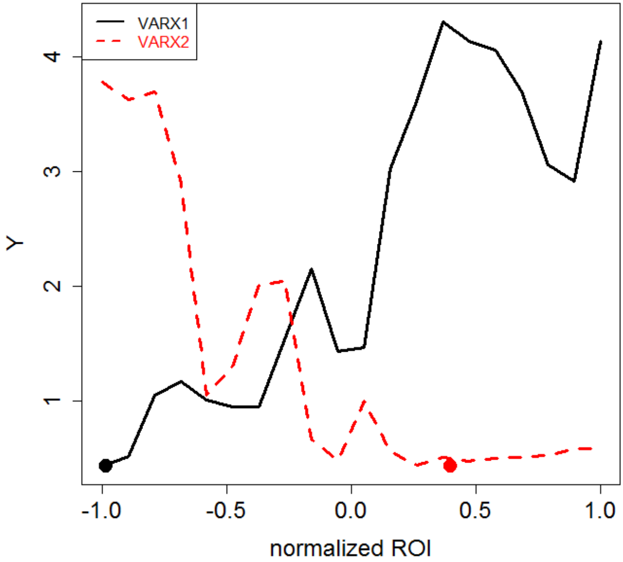
- Output from the following R code:

```
> res<-spot(spotConfig=config,x0=x0,fn=fn,maxit=maxit)

Sensitivity plot for this ROI:
      lower upper type     BEST
VARX1     1   100  INT  1.84744
VARX2     1   100  INT 70.36899

Best solution found with 103 evaluations:
           Y   VARX1    VARX2 COUNT CONFIG
245 0.409769 1.84744 70.36899     5     24

Standard deviation of best solution:
0.409769033349987 +- 0.0112398099327513
```


VARX1
VARX2
Y
4
3
2
1
-1.0
-0.5
0.0
0.5
1.0
normalized ROI

Tuning SANN: Raw Results

- Result file, logged information separated by space

```
Function XDIM YDIM STEP SEED CONFIG VARX1 VARX2 Y
UserSuppliedFunction 2 1 0 1234 1 23 62 0.518342556082896
UserSuppliedFunction 2 1 0 1235 1 23 62 0.402079045134601
UserSuppliedFunction 2 1 0 1234 2 62 33 3.50021485407806
```

- Results in R command line

```
str(res$alg.currentResult)
```

```
'data.frame':   103 obs. of  9 variables:
 $ Function: Factor w/ 1 level "UserSuppliedFunction": 1 1 1
 $ XDIM    : num  2 2 2 2 2 2 2 2 2 2 ...
 $ YDIM    : int  1 1 1 1 1 1 1 1 1 1 ...
 $ STEP    : int  0 0 0 0 0 0 0 0 0 0 ...
 $ SEED    : num  1234 1235 1234 1235 1234 ...
 $ CONFIG  : int  1 1 2 2 3 3 4 4 5 5 ...
 $ VARX1   : num  23 23 62 62 38 38 70 70 8 8 ...
 $ VARX2   : num  62 62 33 33 26 26 16 16 90 90 ...
 $ Y       : num  0.518 0.402 3.5 16.653 4.774 ...
```

Tuning SANN: Other Report Functions

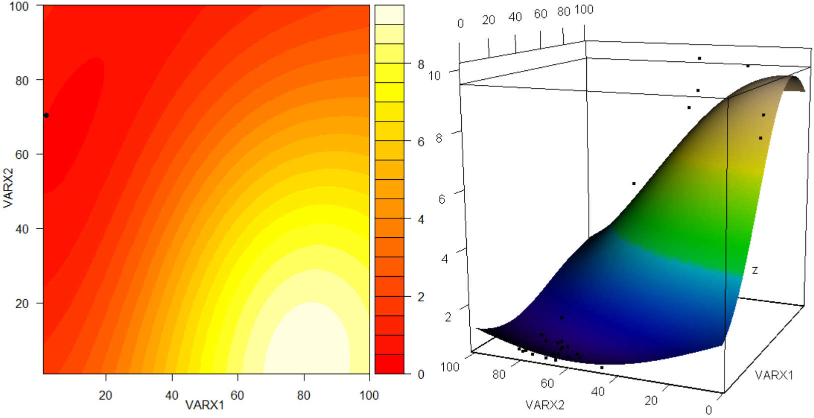
- Other reports/graphics can be created
- spotReportContour for a contour plot

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

- spotReport3d for 3d plot

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

Plots from SPOT



SPOT: Existing Features

- Single and multi criteria optimization
- Automated tuning, or manual steps
- Modular concept: Use different combinations of models / methods
- Available surrogate models: Linear, Tree, Kriging, Support Vector Machine, Random Forest, ...
- Tuning real valued parameters as well as factors (i.e. with tree-based models)
- User can use custom models
- Different means of budget allocation
- Logging and Report generation

Research Topic: Noise Handling

- SPOT provides tools for improving the confidence during the search. First approaches increase the number of repeats. An early SPOT implementation proceeded as follows [4]:

  > *At each step, two new designs are generated and the best is re-evaluated. This is similar to the selection procedure in $(1+2)$-Evolution Strategies. The number of repeat runs, k, of the algorithm designs is increased (doubled), if a design has performed best twice or more. A starting value of $k = 2$ was chosen*

- This simple approach did not use any information about the variance

Selection under Noise: Approaches

- Simple: use an identical number of replications for each design
  - Inefficient, because some designs might have low variance, others high variance
- Efficient: Probability of correct selection (PCS)
  - Definition: Correct selection can be defined as *correctly selecting the true best design*
- Problem variations: Subset selection
  - subset which contains the best
  - subset which contains the m best
  - ...

Selection under Noise: Approaches

- State of the art:
  - allocate a larger portion of the computing budget to design that are critical to the process of identifying the best design
  - Use both: (1) sample means and (2) variances
- Assumptions and Derivation of the OCBA equations (see Appendix)

Research Topic: Noise Handling Using OCBA

- Lasarczyk was the first who combined SPOT and OCBA [9]
- OCBA was developed to ensure a high *probability of correct selection* (PCS)
- To maximize PCS, a larger portion of the available budget is allocated to those designs that are critical to the process of identifying the best candidates
- OCBA uses sample means and variances in the budget allocation procedure in order to maximize PCS

[OCBA's Central Idea]

- A number of simulation replications, say T
- Allocated to m competing design points with means $\overline{Y}_1, \overline{Y}_2, \ldots, \overline{Y}_m$ and finite variances $\sigma_1^2, \sigma_2^2, \ldots, \sigma_m^2$, respectively
- N_i is the number of replications allocated to design i
- $\delta_{b,j} = \overline{Y}_b - \overline{Y}_i$ denotes the difference of the i-th and b-th mean with $\overline{Y}_b \leq \min_{i \neq b} \overline{Y}_i$.

[OCBA's Central Idea]

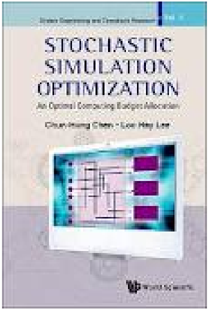
- *Approximate Probability of Correct Selection* asymptotically maximized when

$$\frac{N_i}{N_j} = \left(\frac{\sigma_i/\delta_{b,i}}{\sigma_j/\delta_{b,j}}\right)^2, \quad i,j \in \{1,2,\ldots,m\}, \text{ and } i \neq j \neq b,$$

$$N_b = \sigma_b \sqrt{\sum_{i=1, i\neq b} \frac{N_i^2}{\sigma_i^2}}, \tag{1}$$

OCBA Conclusion

- As can be seen from (1), the allocated computing budget is proportional to variance and inversely proportional to the difference from the best design



SPOT + OCBA: Development

- The OCBA implementation in our study is based on Lasarczyk's work [9]
- New design points which were proposed by the meta model are evaluated several times, e.g., twice [1]
- During each SPOT step, a certain budget (here: `spot.ocba` = 3 is allocated to the candidate solutions to ensure a high PCS for the best design point
- Chen and Lee present a comprehensive coverage of the OCBA methodology [5]

[1] This value can be modified using the `init.design.repeats` variable in SPOT's config file

The OCBA Interface in SPOT

- Spreads the budget in an optimal way for the different design points, considering a minimization problem
- `spotOcba <- function(samp.mean, samp.var, samp.count, budget.add, iz=NA, verbose=0)`
- param
  - samp.mean vector of mean values, length nd
  - samp.var vector of variances, length nd
  - samp.count vector of repeats performed already, length nd
  - budget.add additional number of repeats, distributed among the nd design points
  - iz indifference zone
  - verbose verbosity, 0 is no printing

An OCBA Example in SPOT

```
> samp.mean <- numeric();  samp.var <-  numeric();
> samp.count <- rep(20,10); budget <- 100
> for (m in 1:10) {
+  sample <- rnorm(20, mean=m, sd=6);
+  samp.mean <- c(samp.mean,mean(sample));
+  samp.var <- c(samp.var,var(sample));
+ }
> spotOcba(samp.mean, samp.var, samp.count, budget)
```

```
 [1] 60 40  0  0  0  0  0  0  0  0
```

Current Research

- Extend report functions
- Implementation of ensembles of surrogate models
- Interaction between simulation and surrogate models
- Improve multi criteria optimization
- Adaptive ROI
- New test problems or applications
- Noise handling
- ..., see `www.spotseven.de`
- Discussion ⇒ Cooperation?
  - R source code from the slides

Selection under Noise: Problem Formulation

- Goal: $\min_\theta J(\theta)$, where θ p dimensional vector of (decision) variables
- Real-world application: $J(\theta)$ cannot be determined directly
- $J(\theta) = E[L(\theta, \omega)]$, ω comprises uncertainty
- $L(\theta, \omega)$ available via simulation
- Optimization goal (search):

$$\min \overline{J}(\theta) = \frac{1}{N} \sum_{j=1}^{N} L(\theta, \omega)$$

Critical Designs and OCBA

- General: First step: generate n_0 simulation replications
- Notation summary
    - J_i: true mean of design i
    - σ_i^2: variance of design i
    - $L(\Theta_i, \omega_{ij})$: performance estimate obtained from the output of the jth simulation replication for design i
    - N_i: number of repeats for design i
    - $\overline{J}_i(\theta)$: sample mean of design i, i.e., $(\frac{1}{N_i}\sum_{j=1}^{N_i} L(\theta_i, \omega_{ij})$
    - t: true best design, i.e., $t = \text{argmin}_i J_i$
    - $\delta_{t,i}$: distance ith and best, i.e., $\delta_{t,i} = J_t - J_i$
    - $\sigma_{t,i}^2$: sum of variances, i.e., $\frac{\sigma_t^2}{N_t} + \frac{\sigma_i^2}{N_i}$

OCBA Assumptions

- Simulation output is independent identical distributed and has normal distribution with mean J_i and variance σ_i^2
- $L(\theta_i, \omega_{ij}) \sim N(J_i, \sigma_i^2)$ with known J_i, σ_i^2 and t
- OCBA goal: Find a budget allocation that maximizes PCS, where CS is defined as picking the best design based on sample means from simulation output
- PCS defined as the probability that the true best design has the smallest sample mean and therefore can be selected correctly:

$$PCS = P\{CS\} = P\{\bar{J}_t < \bar{J}_i, i \neq t\}$$

OCBA Assumptions

- Considering normality assumptions $\Rightarrow \overline{J}_i \sim N(J_i, \frac{\sigma_i^2}{N_i})$
- OCBA restated: How should N_i be increased that PCS is maximized $\Rightarrow$ Choose $N_1, N_2, \ldots, N_k$ such that PCS is maximized subject to the budget T (limited)
- $$\max_{N_1,\ldots,N_k} PCS \text{ s.t. } \sum^k N_i = T \qquad (2)$$

OCBA Derivation

- No close-form expression for PCS ⇒ approximation via Bonferroni inequality

$$PCS = P\{\bigcap_{i \neq t} \left(\bar{J}_t - \bar{J}_i < 0\right)\}$$

$$\geq 1 - \sum_{i \neq t}^{k} P\{\bar{J}_t > \bar{J}_i\} =: APCS$$

OCBA Derivation

- Approximation for Eq. 2:

$$\max_{N_1,\ldots,N_k} 1 - \sum_{i \neq t}^{k} P\{\bar{J}_t > \bar{J}_i\} \text{ s.t. } \sum^{k} N_i = T$$

$\Rightarrow$

- Lagrange
- assumption: $N_t >> N_i$
- $T \to \infty$

$\Rightarrow$ Theorem:

OCBA Derivation

- Given a total number of simulation replications T to be allocated to k competing designs with with means $\overline{Y}_1, \overline{Y}_2, \ldots, \overline{Y}_k$ and finite variances $\sigma_1^2, \sigma_2^2, \ldots, \sigma_k^2$, respectively. The *Approximate Probability of Correct Selection* can be asymptotically maximized when

$$\frac{N_i}{N_j} = \left(\frac{\sigma_i / \delta_{b,i}}{\sigma_j / \delta_{b,j}} \right)^2, \quad i, j \in \{1, 2, \ldots, k\}, \text{ and } i \neq j \neq b, \tag{3}$$

$$N_b = \sigma_b \sqrt{\sum_{i=1, i \neq b} \frac{N_i^2}{\sigma_i^2}},$$

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