

sfb 475: reduction of complexity in multivariate data structures



rPorta An R Package for Analyzing Polytopes and Polyhedra

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Introduction •••••

Motivation

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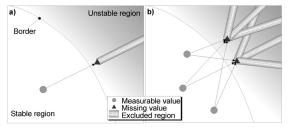
Summary 00

Problem from design of experiments

Generate a space-filling design exploring the unknown feasible parameter space with a minimum of failures/missing values

Strategy (in the spirit of Henkenjohann et al., 2005)

- Assume feasible area is connected and convex
- Viewed from feasible point space behind failure points is failure region
- Examine and restrict parameter space sequentially



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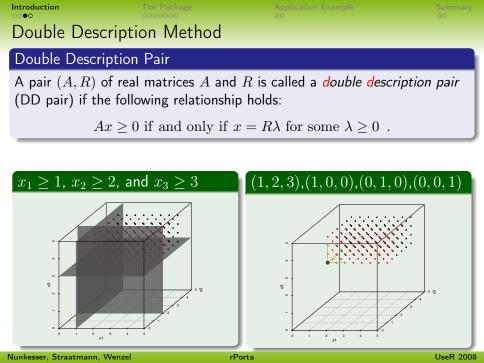
Summary 00

Key aspects required for the strategy in \mathbb{R}^d

- Inefficient to construct a convex cone for each combination of one failure and d feasible points
- Find a fast way to check if a candidate-point is lying inside one of these cones and hence is a failure point

Solution

- Use Polyhedral Convex Cones (PCCs) with *extreme rays* to minimize number of convex cones
- Calculate PCCs with Double Description Method as introduced in Fukuda and Prodon (1996)



Double Description Method

Polyhedral Cone

A subset $P \in \mathbb{R}^d$ is called a *polyhedral cone* if

$$\exists A \in \mathbb{R}^{n \times d} : P = \{x \in \mathbb{R}^d : Ax \ge 0\} =: P(A)$$

Representation and Generation

Let $P \in \mathbb{R}^d$ be a polyhedral cone and $A \in \mathbb{R}^{n \times d}$ be the matrix with P = P(A). Then there exists a matrix $R \in \mathbb{R}^{d \times m}$ such that (A, R) is a DD pair and it is:

$$P = \{x \in \mathbb{R}^d : Ax \ge 0\}$$

= $\{x \in \mathbb{R}^d : x = R\lambda \text{ for some } \lambda \ge 0\}$

A is called *representation matrix* of the polyhedral cone P, R is called *generating matrix* for the polyhedral cone.

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R Package rPorta

R Interface to PORTA (Polyhedron Representation Transformation Algorithm) by T. Christof (Universität Heidelberg) and A. Löbel (ZIB)

What is PORTA?

- Collection of routines for analyzing polytopes and polyhedra
- Supports both representations of the double description pair
- Transforms between the representations

Why PORTA? (and not polymake, cdd, PPL,...)

- Platform independence (gcc)
- Free availability (GPL license)
- Speed
- Fitting functionality for the intended application

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Comparison to rcdd

rcdd is an R Package interfacing cdd(lib) (C implementation of the double description method) by K. Fukuda (Swiss Federal Institute of Technology)

What is cdd?

- · Supports both representations of the double description pair
- Transforms between the representations
- Additionaly solves linear programming problems

Short comparison

Point of	rPorta	rcdd		
comparison				
Platforms	Every platform with R	Every platform with gmp		
Arithmetic	64 bit rational arithmetic	Exact rational arithmetic		
Functions	Collection for transforming and analyzing polyhedra	Focuses on transformation and linear programming		

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Summary

PORTA's UI and its R Counterpart

PORTA reads all data from and to files \leftrightarrow rPorta wraps files into S4 classes

Example of an ieq file $(\hat{=} representation matrix A)$	S4 object ieqExample $(\hat{=} representation matrix A)$
DIM = 3	> ieqExample@inequalities@num
	[,1] [,2] [,3] [,4]
INEQUALITIES_SECTION	[1,] 1 0 0 1
(1) x1 >= 1	[2,] 0 1 0 2
(2) x2 >= 2	[3,] 0 0 1 3
(3) x3 >= 3	
	>ieqExample@inequalities@sign
END	[1] 1 1 1

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PORTA's UI and its R Counterpart

PORTA reads all data from and to files \leftrightarrow rPorta wraps files into S4 classes

Example of a poi file $(\hat{=} \text{ generating matrix } R)$	S4 object poiExample $(\hat{=} \text{ generating matrix } R)$
DIM = 3	> poiExample=traf(ieqExample)
CONV_SECTION	<pre>> poiExample@convex_hull@num</pre>
1 2 3	[,1] [,2] [,3]
	[1,] 1 2 3
CONE_SECTION	
0 0 1	<pre>> poiExample@convex_cone@num</pre>
0 1 0	[,1] [,2] [,3]
1 0 0	[1,] 0 0 1
	[2,] 0 1 0
END	[3,] 1 0 0

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Method traf

Method to transform between the double description pair representations

S4 method

traf(object, opt_elim=FALSE, chernikov_rule_off=FALSE, validity_table_out=FALSE, long_arithmetic=FALSE)

object Object of class ieqFile or poiFile

opt_elim Use a heuristic to eliminate that variable next, for which the number of new inequalities is minimal

validity_table_out Include a table which indicates strong validity

long_arithmetic Use long integers for intermediate results

Example for traf

> poiExample=traf(ieqExample)

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Method fctp

Checks the facet inducing property

S4 method

fctp(object, poiObject)

object, poiObject ieqFile object and poiFile object to check

Example ieqFile	Result for $(0,1,0)$, $(0,0,2)$, and $(0,0,3)$
DIM = 3	[[1]] # not valid for (1)
VALID	0 1 0
2 0 0	<pre>[[2]] # satisfying (1) with equality</pre>
INEQUALITIES_SECTION	0 0 2
(1) $x1 + x2 + x3 \ge 2$	[[3]] # not valid for (2)
(2) $x1 + x2 + x3 \le 2$	0 0 3
(3) x1 >= 0	<pre>[[4]] # satisfying (2) with equality</pre>
(4) x2 >= 0	0 0 2
(5) x3 >= 0	

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Some Other Functions

Helper functions

as.poi, as.ieq turns objects into poi or ieq objects

read.portaFile converts PORTA files to corresponding S4 classes

PORTA functions

vint enumerates integral points of a linear system
portsort sorts and formats poiFile and ieqFile objects
fmel projects a linear system to a subspace
iespo enumerates valid inequalities for a given polyhedron
posie enumerates valid points for given inequalities

Application specific functions

failureRegions function specific for the application example

Application of rPorta

failureRegions determines unfeasible regions inside a parameter space (here: 3 steps with 10 points each to restrict parameter space $[-2,2]^2$)

S4 method

failureRegions(experiments, parameterspace, fail)

parameterspace Represents parameter space grid (here: 1681 points)
 experiments Contains the points with known results (here: initial 10
 point uniform coverage design)

fail A logical vector indicating which experiments failed

res <- failureRegions(as.poi(exper),as.poi(paramspace),fails)
restrictedSpace <- as.matrix(getFeasiblePoints(res))</pre>

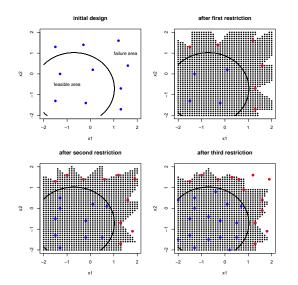
- update with 10 new points from restrictedSpace regarding space-filling criterias
- restrict restrictedSpace again (repeat until 3 restrictions)

Result

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rPorta	
Each step < 1 second	

Old Method

Step 1:	16.6 seconds
Step 2:	194.17 seconds
Step 3:	744.01 seconds

Summary

- Double Description Method speeds up handling of convex cones
- rPorta provides an interface to a double description implementation
- Easy analysis of polytopes and polyhedra in R



- Fukuda, K., Prodon, A., 1996. Double description method revisited. In: Combinatorics and Computer Science. Vol. 1120 of LNCS. Springer-Verlag, London, pp. 91–111.
- Geyer, C. J., Meeden, G. D., 2008. rcdd: rcdd (C Double Description for R). R package version 1.1.
- Henkenjohann, N., Göbel, R., Kleiner, M., Kunert, J., 2005. An adaptive sequential procedure for efficient optimization of the sheet metal spinning process. Quality and Reliability Engineering International 21 (5), 439–455.
- Nunkesser, R., Straatmann, S., Wenzel, S., 2008. rPorta: R/PORTA interface. R package version 0.1-6.