BEUTH HOCHSCHULE FÜR TECHNIK BERLIN
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Design of Experiments in R

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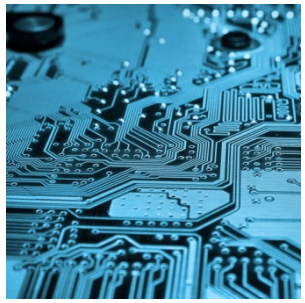

Outline of presentation

Design of Experiments (DoE) in *R*

- An introductory example
  and the principles of (industrial) DoE
- DoE in ***R***: what is there?
- Development of my package suite
  for (industrial) DoE in ***R***
- GUI: conceptual questions
- Call for activities

An example: Car seat occupation

An example: Car seat occupation

Example: Car seat occupation

- Mat (sensor cells) and detection algorithm decide, whether airbag opens
  Requirements:
  - Must open for adult normal or heavy passenger (critical)
  - Must not open for small child (critical)
  - Must not open for rearward facing child seat (critical)
  - Should not open for empty seat
  - Should not open for objects not worthy of protection (box)
- System must work reliably under all expected seat conditions; experiment to understand which factors are critical
  - Foam hardness (hard / soft)
  - Side bolster stiffness (stiff / soft)
  - Aging (new / aged)
  - ... (a total of six 2-level factors)
- Target variables: measurement results from defined dummies

Example: Car seat occupation

- Questions to be answered for an experimental design
  - Which type of design?
    Unconfounded estimation of main effects and 2-factor interactions
    - 32 run regular fractional factorial (resolution VI)
  - Established process for measuring the response?
    - Here: measuring depends on placement of dummy,
      thus repeat three times with reseating dummy inbetween
  - Are 32 runs enough (precision considerations)?
    - Yes (with repeating seating of dummies, as indicated above)
  - Can 32 runs be afforded (economical considerations)?
    - Yes

Example: Car seat occupation

run	Foam	Bolster	Aged	D	E	F	run	Foam	Bolster	Aged	D	E	F
20	soft	soft	new	-	-	-	31	soft	soft	new	-	+	+
19	hard	soft	new	-	-	+	15	hard	soft	new	-	+	-
14	soft	stiff	new	-	-	+	8	soft	stiff	new	-	+	-
25	hard	stiff	new	-	-	-	24	hard	stiff	new	-	+	+
5	soft	soft	aged	-	-	+	27	soft	soft	aged	-	+	-
17	hard	soft	aged	-	-	-	32	hard	soft	aged	-	+	+
12	hard	stiff	new	+	-	+	10	hard	stiff	new	+	+	-
26	soft	soft	aged	+	-	-	29	soft	soft	aged	+	+	+
30	hard	soft	aged	+	-	+	11	hard	soft	aged	+	+	-
13	soft	stiff	aged	+	-	+	23	soft	stiff	aged	+	+	-
1	hard	stiff	aged	+	-	-	28	hard	stiff	aged	+	+	+

```
plan <-
FrF2(32, 6, factor.names=list(Foam=c("soft","hard"),
     Bolster=c("soft","stiff"),Aged=c("new","aged"),
     D=c("-","+"),E=c("-","+"),F=c("-","+")),
     seed=27865)
```

Example: Car seat occupation

run	Foam	Bolster	Aged	D	E	F	run	Foam	Bolster	Aged	D	E	F
20	soft	soft	new	-	-	-	31	soft	soft	new	-	+	+
19	hard	soft	new	-	-	+	15	hard	soft	new	-	+	-
14	soft	stiff	new	-	-	+	8	soft	stiff	new	-	+	-
25	hard	stiff	new	-	-	-	24	hard	stiff	new	-	+	+
5	soft	soft	aged	-	-	+	27	soft	soft	aged	-	+	-
17	hard	soft	aged	-	-	-	32	hard	soft	aged	-	+	+
2	soft	stiff	aged	-	-	-	21	soft	stiff	aged	-	+	+
4	hard	stiff	aged	-	-	+	9	hard	stiff	aged	-	+	-
22	soft	soft	new	+	-	+	18	soft	soft	new	+	+	-
7	hard	soft	new	+	-	-	3	hard	soft	new	+	+	+
16	soft	stiff	new	+	-	-	6	soft	stiff	new	+	+	+
12	hard	stiff	new	+	-	+	10	hard	stiff	new	+	+	-
26	soft	soft	aged	+	-	-	29	soft	soft	aged	+	+	+
30	hard	soft	aged	+	-	+	11	hard	soft	aged	+	+	-
13	soft	stiff	aged	+	-	+	23	soft	stiff	aged	+	+	-
1	hard	stiff	aged	+	-	-	28	hard	stiff	aged	+	+	+

Design in run order

	Foam	Bolster	Aged	D	E	F
1	hard	stiff	aged	+	-	-
2	soft	stiff	aged	-	-	-
3	hard	soft	new	+	+	+
4	hard	stiff	aged	-	-	+
5	soft	soft	aged	-	-	+
6	soft	stiff	new	+	+	+
7	hard	soft	new	+	-	-
8	soft	stiff	new	-	+	-
9	hard	stiff	aged	-	+	-
10	hard	stiff	new	+	+	-
11	hard	soft	aged	+	+	-
12	hard	stiff	new	+	-	+
13	soft	stiff	aged	+	-	+
14	soft	stiff	new	-	-	+
15	hard	soft	new	-	+	-
16	soft	stiff	new	+	-	-

	Foam	Bolster	Aged	D	E	F
17	hard	soft	aged	-	-	-
18	soft	soft	new	+	+	-
19	hard	soft	new	-	-	+
20	soft	soft	new	-	-	-
21	soft	stiff	aged	-	+	+
22	soft	soft	new	+	-	+
23	soft	stiff	aged	+	+	-
24	hard	stiff	new	-	+	+
25	hard	stiff	new	-	-	-
26	soft	soft	aged	+	-	-
27	soft	soft	aged	-	+	-
28	hard	stiff	aged	+	+	+
29	soft	soft	aged	+	+	+
30	hard	soft	aged	+	-	+
31	soft	soft	new	-	+	+
32	hard	soft	aged	-	+	+

class=design, type= FrF2

Principles of DoE

- Historical: R.A.Fisher in early 20th century and some earlier researchers (c.f. e.g. Preece 1990) brought forward central principles

- ***Block*** *what you can and* ***randomize*** *what you cannot*
  (Box, Hunter and Hunter 1978; 2005)
  - **Randomization**: balance out unknown influences
  - **Blocking**: balance out known influences, reduce error variability

- **Replication**: don‘t generalize one-offs
  - ***Repeated measurements*** *are* ***NOT*** *replications*
  - Balanced factorial experiments provide intrinsic replication
    → more efficient than one-factor-at-a-time comparisons

- **Analysis follows design!**
  for example also for split-plot designs

Principles of DoE

George Box (Fisher's son-in-law) and colleagues during 20th century

- Proceed **sequential**ly
  - smaller initial screening experiments
  - response surface experiments with few relevant factors later; second-order approximation will often be good

In late 20th century,
the different nature of computer experiments was recognized and catered for:

- **Computer experiments** have different needs, e.g. no use for replication
  e.g. Sacks et al. 1989 Statistical Science

  space-filling designs

Jump to next topic

Car seat example

	Foam	Bolster	Aged	D	E	F		Foam	Bolster	Aged	D	E	F
1	hard	stiff	aged	+	-	-	17	hard	soft	aged	-	-	-
2	soft	stiff	aged	-	-	-	18	soft	soft	new	+	+	-
3	hard	soft	new	+	+	+	19	hard	soft	new	-	-	+
4	hard	stiff	aged	-	-	+	20	soft	soft	new	-	-	-
5	soft	soft	aged	-	-	+	21	soft	stiff	aged	-	+	+
6	soft	stiff	new	+	+	+	22	soft	soft	new	+	-	+
7	ha										+	+	-
8	so										-	+	+
9	hard	stiff	aged	-	+	-	25	hard	stiff	new	-	-	-
10	hard	stiff	new	+	+	-	26	soft	soft	aged	+	-	-
11	hard	soft	aged	+	+	-	27	soft	soft	aged	-	+	-
12	hard	stiff	new	+	-	+	28	hard	stiff	aged	+	+	+
13	soft	stiff	aged	+	-	+	29	soft	soft	aged	+	+	+
14	soft	stiff	new	-	-	+	30	hard	soft	aged	+	-	+
15	hard	soft	new	-	+	-	31	soft	soft	new	-	+	+
16	soft	stiff	new	+	-	-	32	hard	soft	aged	-	+	+

class=design, type= FrF2

Needs for blocking, repeated measurements or replication may lead to modifications of the design

Example: Car seat occupation

	run.no	run.no.std.rp	Day	Foam	Bolster	Aged	D	E	F
1	1	8.1.8	1	soft	stiff	aged	+	+	-
2	2	4.1.4	1	soft	soft	new	+	+	-
3	3	12.1.12	1	hard	soft	aged	+	+	-
4									+
5									+
6									+
7									-
8									+
9									-
10									+
11									+
12									+
13									-
14									-
15	15	9.1.9	1	hard	soft	aged	-	-	-
16	16	10.1.10	1	hard	soft	aged	-	+	+
	run.no	run.no.std.rp	Day	Foam	Bolster	Aged	D	E	F
17	17	22.2.6	2	soft	stiff	new	-	+	-
18	18	19.2.3	2	soft	soft	aged	+	-	-
19	19	18.2.2	2	soft	soft	aged	-	+	-

Known influence: *two days of experimentation with separate teams of experimenters*

Blocking should be requested
(**`blocks=2, block.name="Day"`**)

- automatic determination of blocks such that good balance *within* each block and *between* blocks
  → blocks don‘t confound effects of interest
- randomization of runs within blocks

back

Example: Car seat occupation

- Plan including the repeated measurements done with a particular dummy

```
   Foam Bolster Aged D E F y.1 y.2 y.3
1  hard   stiff  new - + +  NA  NA  NA
2  hard   stiff aged - - +  NA  NA  NA
3
4
5
6
7
8
9
10
11
12
13
14
15 soft   stiff  new + + +  NA  NA  NA
16 soft   stiff  new - - +  NA  NA  NA
17 soft    soft aged + + +  NA  NA  NA
18 hard   stiff  new + - +  NA  NA  NA
19 hard    soft  new + + +  NA  NA  NA
```

High measurement error expected
from placement of dummies

Repeated Measurements

- in case of high **measurement error** variance
- repeats done directly in sequence for one setup of the experimental run (**`replications=3`**, **`repeat.only=TRUE`**)
- analyze their averages as unreplicated design, or more sophisticated

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Example: Car seat occupation

	Foam	Bolster	Aged	D	E	F		Foam	Bolster	Aged	D	E	F
1	hard	stiff	aged	+	-	-	17	hard	soft	aged	-	-	-
2	soft	stiff	aged	-	-	-	18	soft	soft	new	+	+	-
3	hard	soft	new	+	+	+	19	hard	soft	new	-	-	+
4													
5													
6													
7													
8													
9													
10													
11													
12													
13	soft	stiff	aged	+	-	+	29	soft	soft	aged	+	+	+
14	soft	stiff	new	-	-	+	30	hard	soft	aged	+	-	+
15	hard	soft	new	-	+	-	31	soft	soft	new	-	+	+
16	soft	stiff	new	+	-	-	32	hard	soft	aged	-	+	+

class=design, type= FrF2

Suppose we had found that
„96 runs are needed for precision“ and affordable.
That would imply 3 replications instead of three repeated measurements.

Replications – very different from repeated measurements!

- ensure sufficient precision of the experiment
- have to replicate **all sources of variability**
- run in separate blocks
  (**replications=3**, **repeat.only=FALSE**)

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DoE in *R*: What is there?

Thanks to Achim Zeileis for providing CRAN Task Views !
http://cran.r-project.org/web/views/

CRAN Task View (http://cran.r-project.org/web/views/ExperimentalDesign.html)
„Design of Experiments and Analysis of Experimental Data“
(or brief: Experimental Design)

- started February 2008
- currently contains 37 ***R*** packages related to Design of Experiments
- Main purposes
  - Pointer to existing functionality
  - support synergies, avoid double work
- Maintainers need help (cf. also Fox 2009): please
  - point out relevant packages
  - or – perhaps occasionally – complain about packages in a task view that are not helpful

DoE in *R*: What is there?

CRAN packages in the view

- 2000 conf.design (**core**) (d)
- 2003 ldDesign
- 2004 AlgDesign (**core**)
- 2004 crossdes (d)
- 2004 BsMD (a)
- 2005 BHH2
- 2005 qtlDesign (d)
- 2005 SensoMineR
- 2006 agricolae (**core**)
- 2006 lhs (d)
- 2007 blockTools (d)
- 2007 desirability (a)
- 2007 experiment
- 2007 FrF2 (**core**) (design 2009)
- 2007 granova (a)
- 2008 rsm (**core**)
- 2009 DoE.base (**core**)
- 2009 DoE.wrapper (**core**)
- 2009 gsDesign
- 2009 RcmdrPlugin.DoE
- 2010 DoseFinding (prior 2008)
- 2010 dae
- 2010 DiceDesign (d)
- 2010 DiceEval (a)
- 2010 DiceKriging (a)
- 2010 DiceView (a)
- 2010 FrF2.catlg128 (d)
- 2010 GAD (a)
- 2010 mkssd (d)
- 2010 qualityTools
- 2010 TEQR
- 2011 mxkssd (d)
- 2011 odprism (d)
- 2011 osDesign
- 2011 asd (d)
- 2011 support.CEs
- 2011 Vdgraph (a)

DoE in *R*: What is there?

Packages for special applications

CRAN packages in the view

- 2000 conf.design (**core**) (d)
- 2003 ldDesign
- 2004 AlgDesign (**core**)
- 2004 crossdes (d)
- 2004 BsMD (a)
- 2005 BHH2
- 2005 qtlDesign (d)
- 2005 SensoMineR
- 2006 agricolae (**core**)
- 2006 lhs (d)
- 2007 blockTools (d)
- 2007 desirability (a)
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- 2011 odprism (d)
- 2011 osDesign
- 2011 asd (d)
- 2011 support.CEs
- 2011 Vdgraph (a)

DoE in *R*: What is there ?

Packages for computer experiments

CRAN packages in the view

- 2000 conf.design (**core**) (d)
- 2003 ldDesign
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DoE in *R*: What is there ?

Packages for general multifactor experiments

CRAN packages in the view

- 2000 conf.design (**core**) (d)
- 2003 ldDesign
- 2004 AlgDesign (**core**)
- 2004 crossdes (d)
- 2004 BsMD (a)
- 2005 BHH2
- 2005 qtlDesign (d)
- 2005 SensoMineR
- 2006 agricolae (**core**)
- 2006 lhs (d)
- 2007 blockTools (d)
- 2007 desirability (a)
- 2007 experiment
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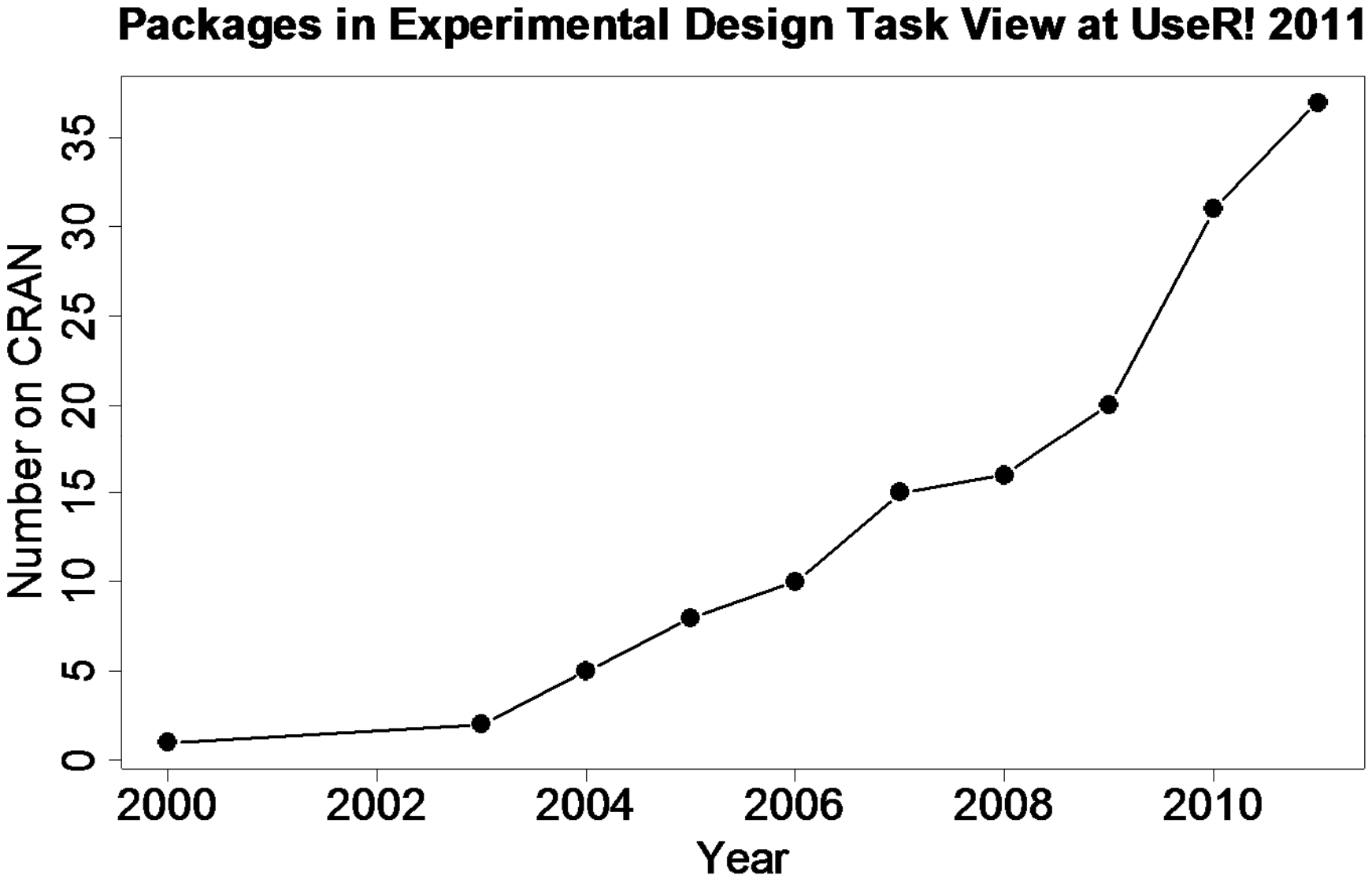
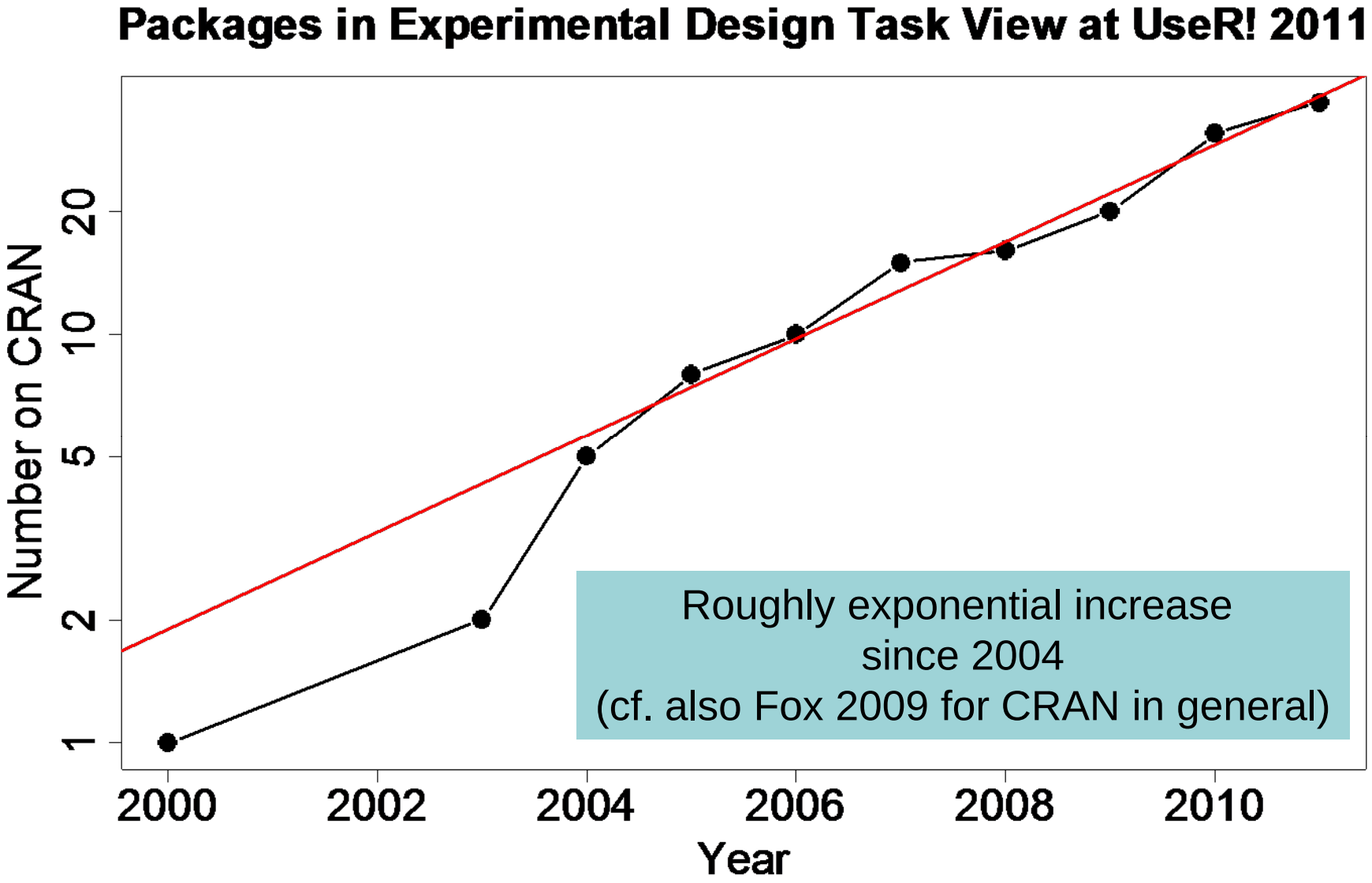
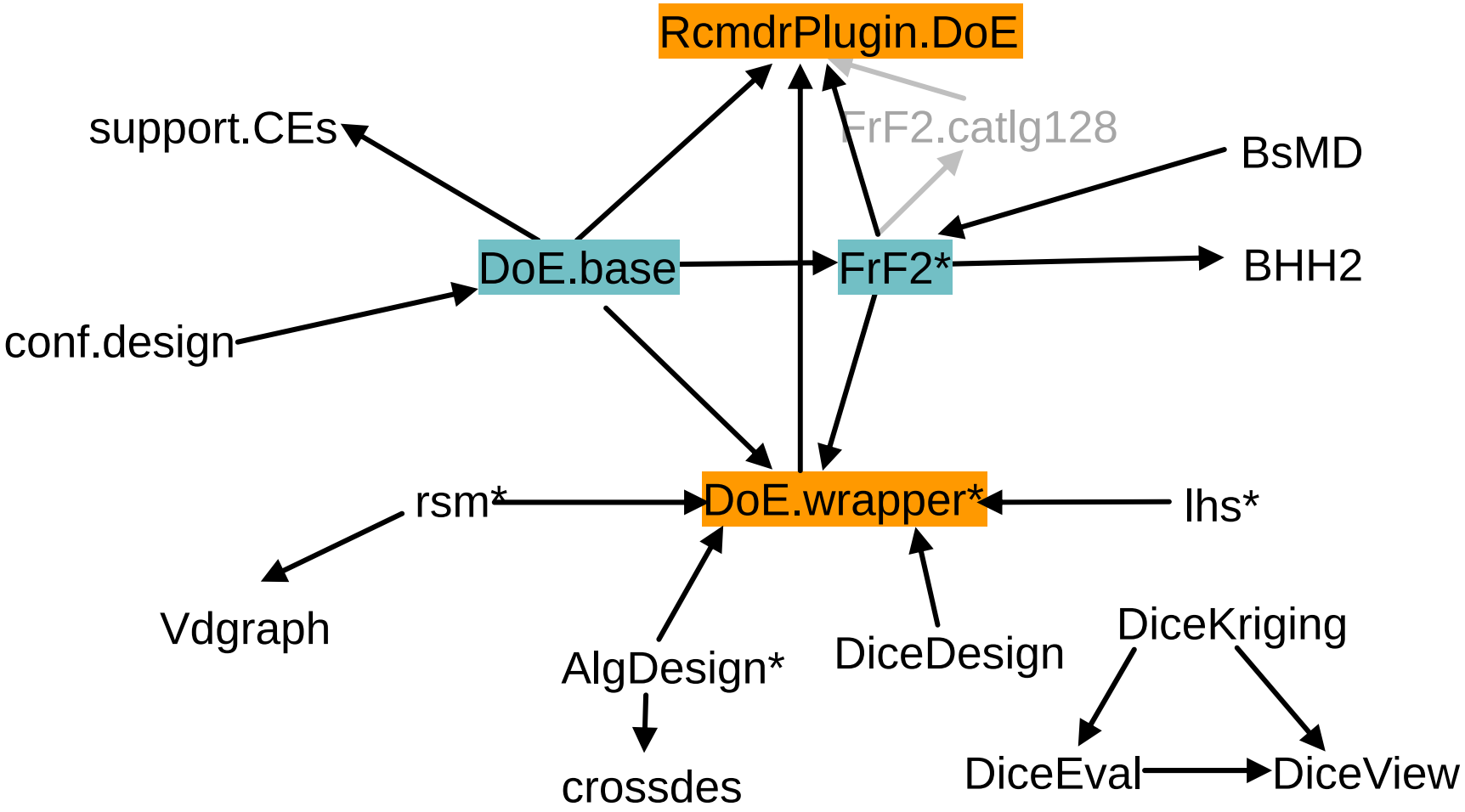
R embraces DoE



R embraces DoE



Relations among DoE packages

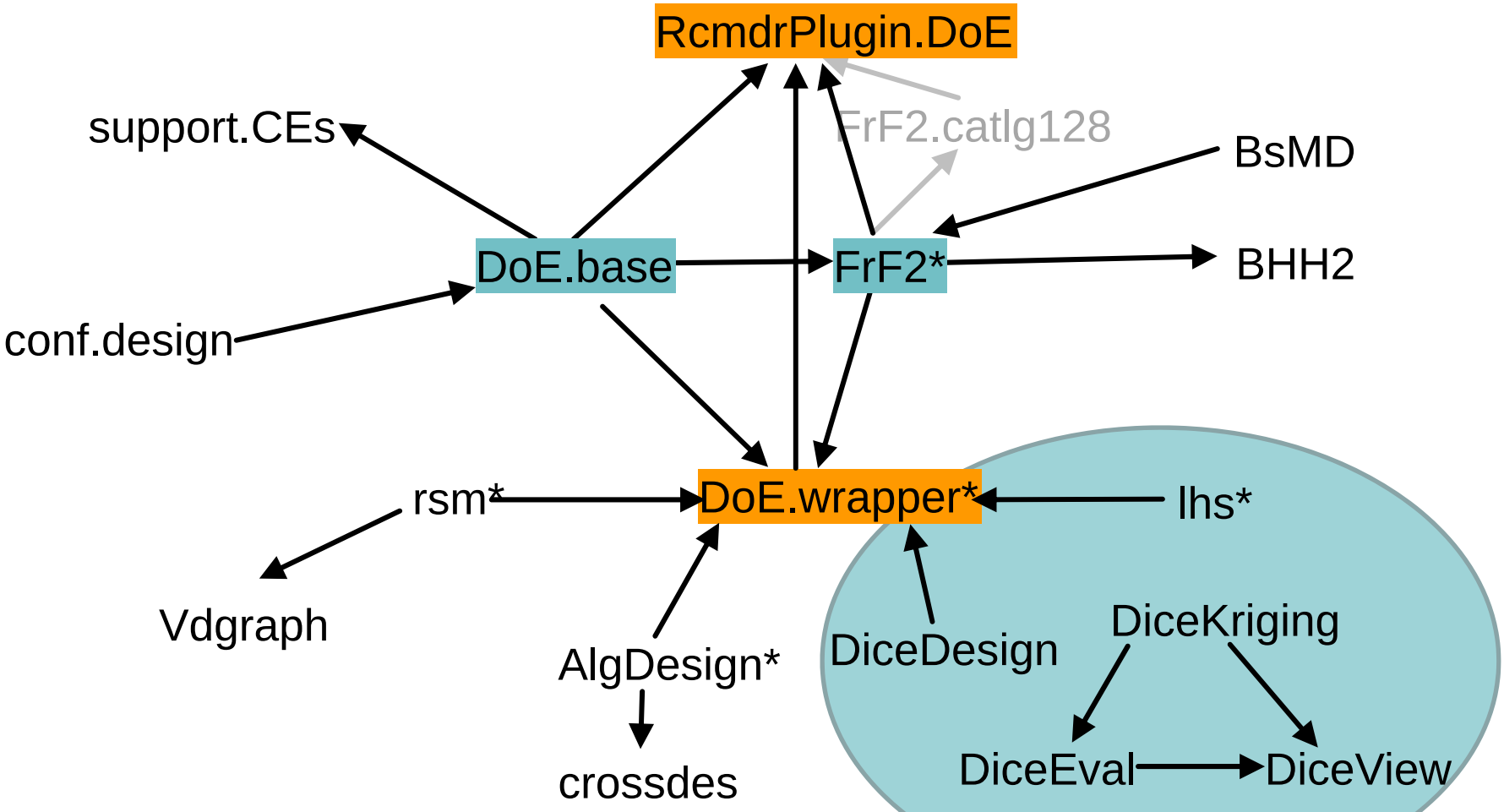


18 of 37 packages have a dependency relation to others.

A → B: B directly depends on or suggests A

*package suggested by SPOT

Relations among DoE packages



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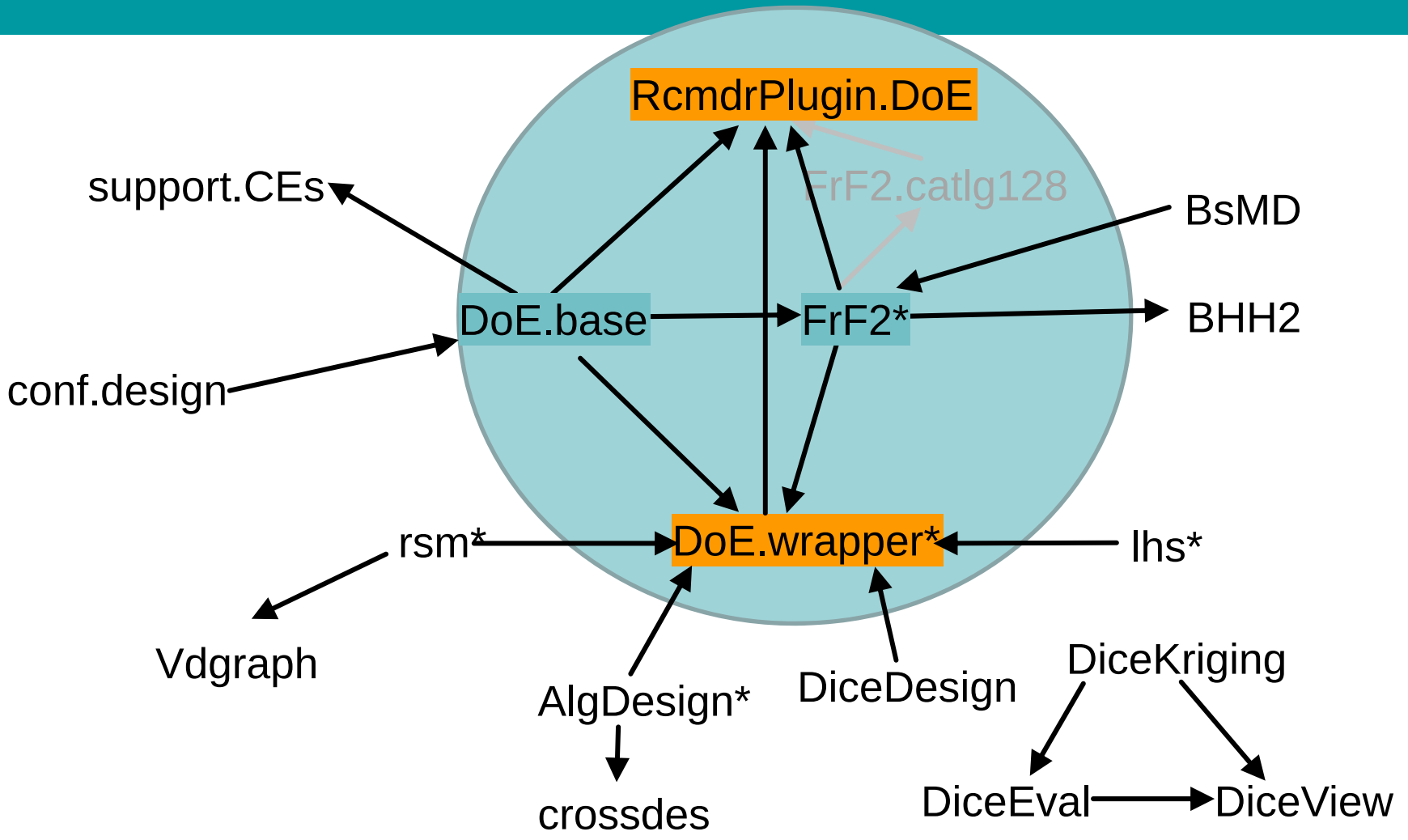
Relations among DoE packages



18 of 37 packages have a dependency relation to others.

A → B: B directly depends on or suggests A

*package suggested by SPOT

Development of my package suite

What made me work on DoE in *R* ?

- Key driver
  - wanted free software solution for industrial experimentation
  - Most often needed: fractional factorial 2-level designs (→**FrF2**)
  - Also sometimes needed: orthogonal arrays (→**DoE.base**)
- Status of DoE possibilities in ***R*** in 2008:
  - almost ***nothing convenient*** for those purposes
  - functions **`fac.design`** and **`oa.design`** from the „White Book“ (Chambers and Hastie 1993) not in ***R***
  - explicit creation of regular fractional factorial 2-level designs, only by specifying generators (packages **BHH2** and **conf.design**)
    - heavy work left to the user, who must work out the generators
  - Package **AlgDesign** would generate regular fractional factorial 2-level designs as D-optimal designs, but often not quite

Mission

Free researchers‘ and experimenters‘ brains

From intricate mathematical and/or programming tasks

For thinking about the application problem

Package suite for industrial DoE in *R*

Package **DoE.base** **(„medium“ to „mature“ version on CRAN, 0.22-5)**
for full factorials with blocking (**`fac.design`**),
orthogonal arrays (**`oa.design`**),
and infrastructure for the other packages

conf.design
relimp
vcd

Package **FrF2** **(„mature“ version on CRAN, 1.2-8)**
for (regular and non-regular) 2-level fractional factorials
FrF2.catlg128 supports

BsMD
igraph
scatterplot3d
sfsmisc

Package **DoE.wrapper** **(„medium“ version on CRAN, 0.8-3)**

- wrapper for existing functionality
  to unify syntax and output structure (class **`design`**)
  and add comfort where necessary
- Basis for including external functionality into GUI package

AlgDesign
DiceDesign
lhs
rsm

GUI interface as an **R-commander plugin** **Version 0.11-2** :
Package **RcmdrPlugin.DoE** **(„early“ version on CRAN)**

Rcmdr

Common syntax

- Partly picked up from the „White book“
- Most design generating functions have parameters
  `nruns, nfactors, factor.names,`
  `replications, repeat.only,`
  `randomize, seed`
- **`FrF2`** and **`fac.design`** have options for blocking
  `blocks`, **`block.name`**, **`block.gen`**, **`bbreps`**, **`wbreps`**
- Generally reasonable defaults
  → only few parameters have to be specified
  e.g.,
  `FrF2` has 33 parameters, most can be omitted most of the time

```
FrF2(32, 6)

FrF2(nfactors=6, resolution=5)
```

Common output structure

- Data frame object of S3 class **`design`**
  - has been inspired by the White Book (Chambers and Hastie 1993): a **data frame with attributes**
    - the data frame itself: the design as factors or uncoded data
    - three attributes
      - **`desnum`**: numeric or coded version of the design (model matrix)
      - **`run.order`**: data frame with run order information
        - used for switching between standard and randomized order
      - **`design.info`**: list with design type-dependent information
        - used extensively by methods for class **`design`**
- Methods for printing, summarizing, plotting, linear model analysis
- Functions for exporting, adding a response, effects plots, ...

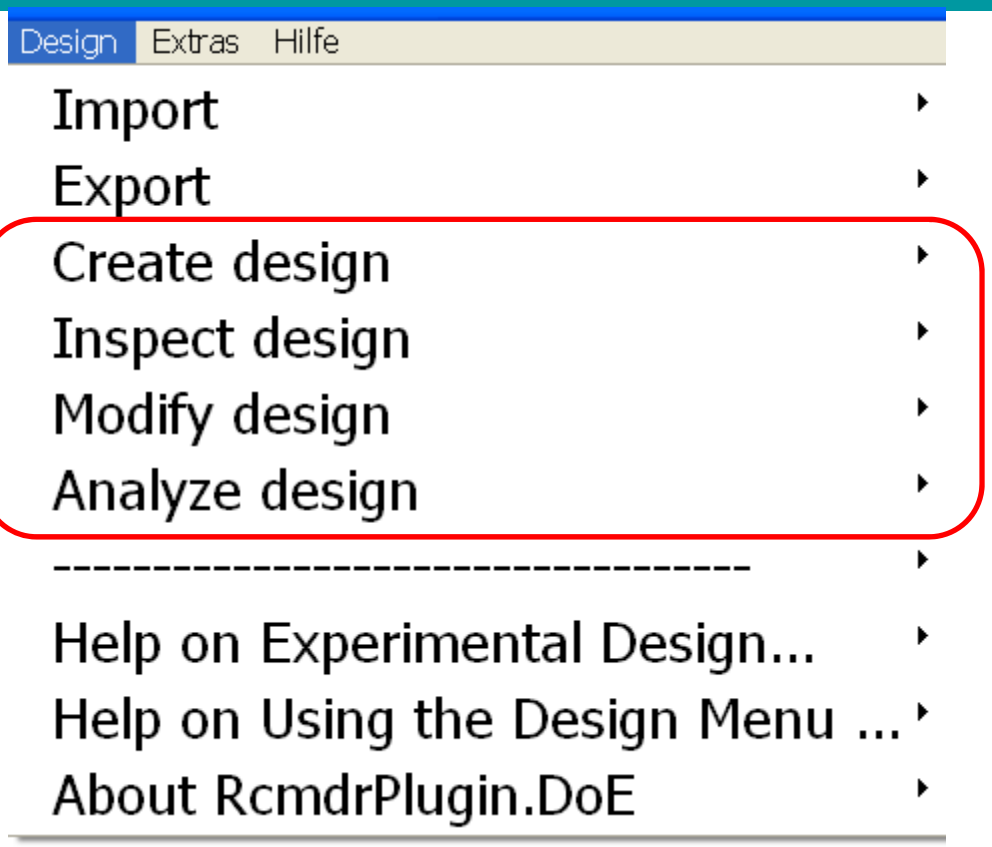
Mission

Free researchers‘ and experimenters‘ brains

From intricate mathematical and/or programming tasks

For thinking about the application problem

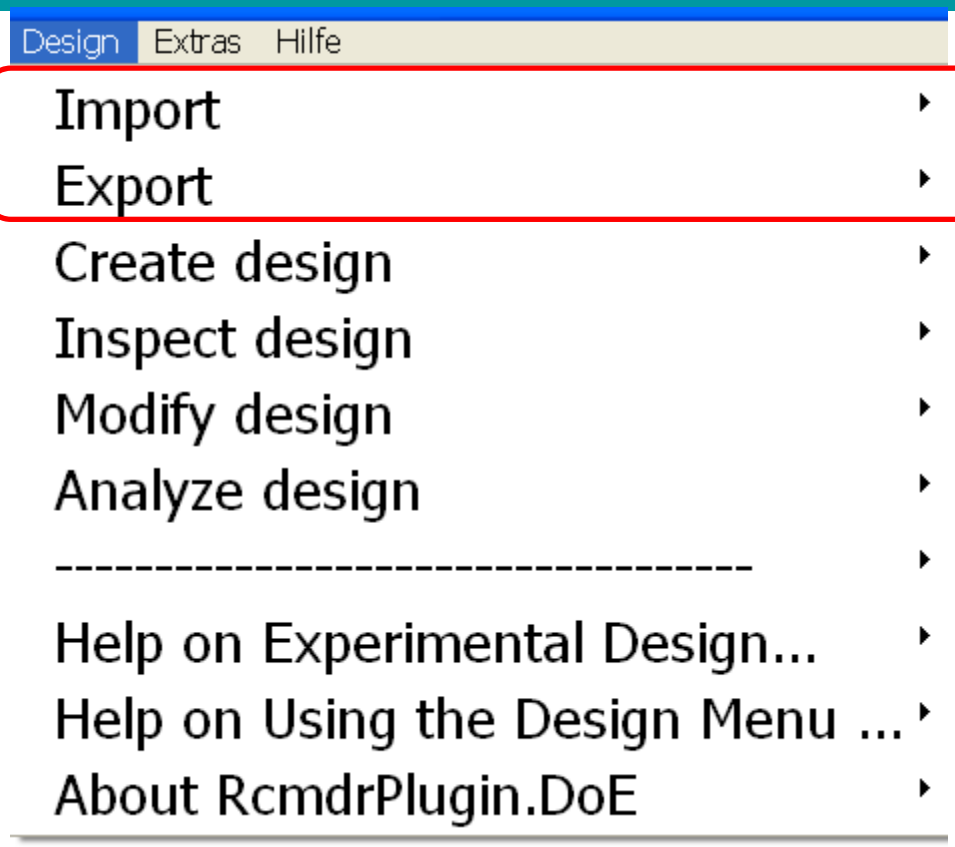
The GUI concept: simplicity



Simple steps

RcmdrPlugin.DoE
plugin for ***R*** Commander (tcltk)

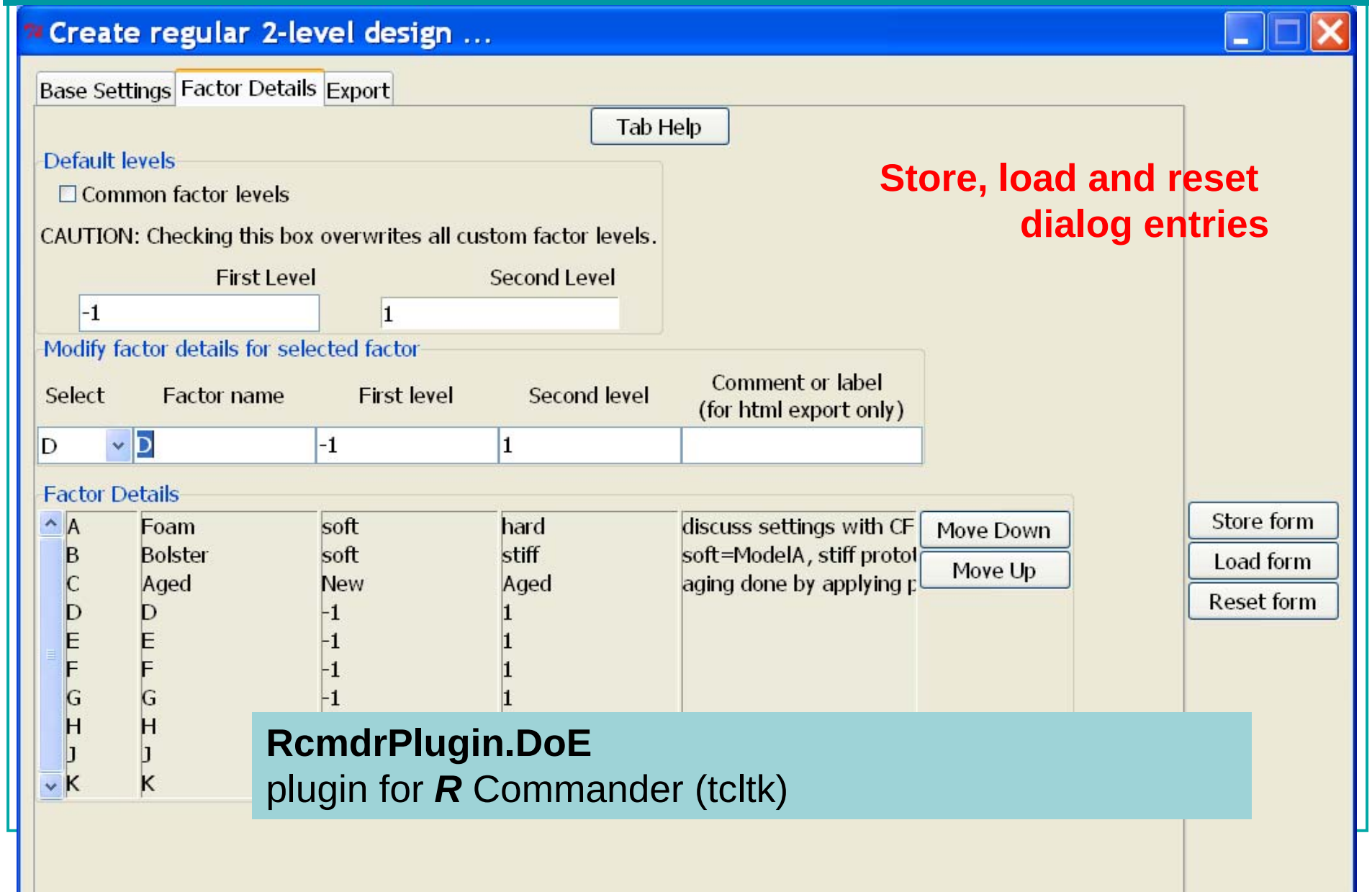
The GUI concept: usability



Import and export
e.g. to spreadsheet

RcmdrPlugin.DoE
plugin for ***R*** Commander (tcltk)

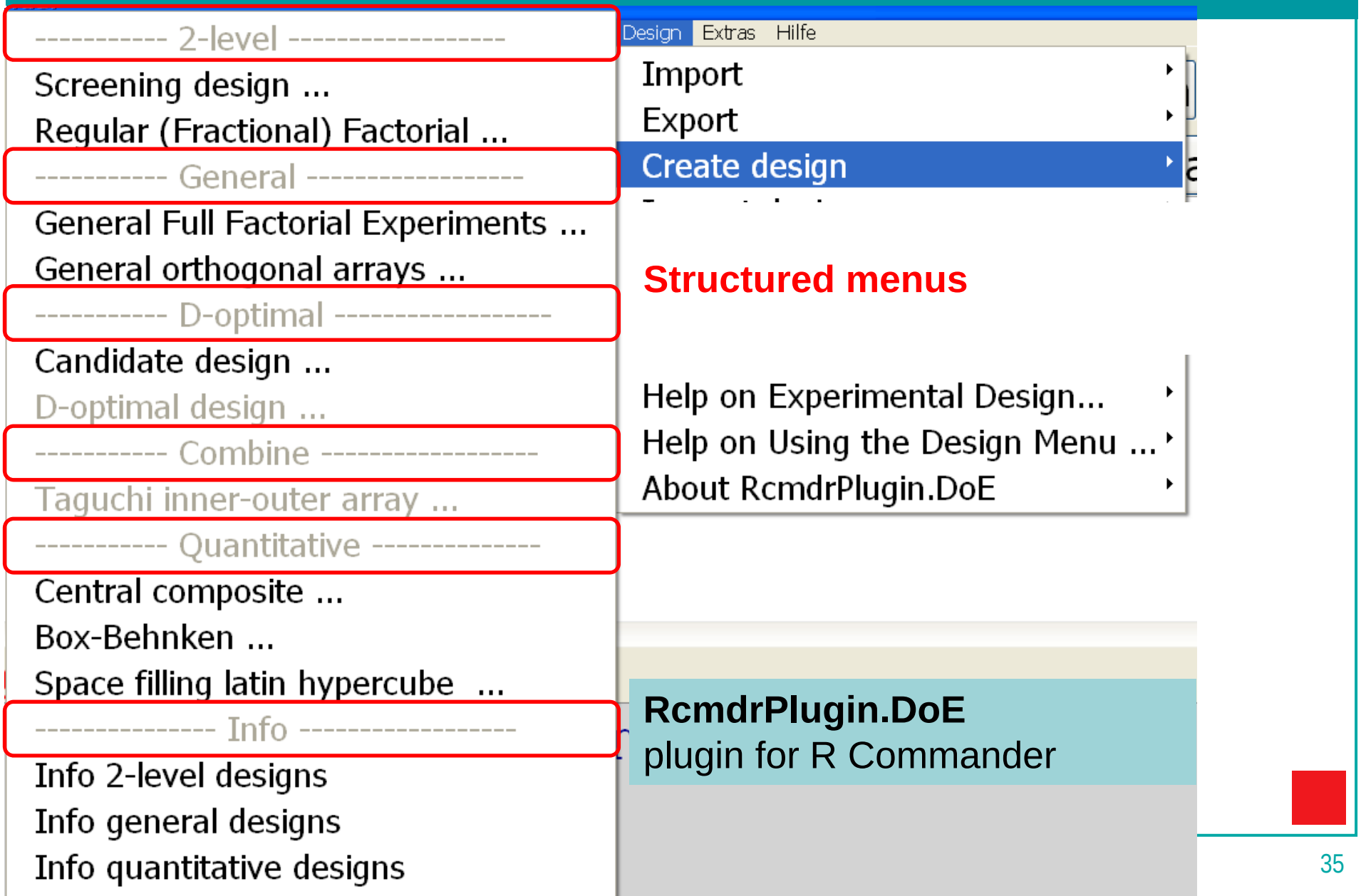
GUI concept: usability



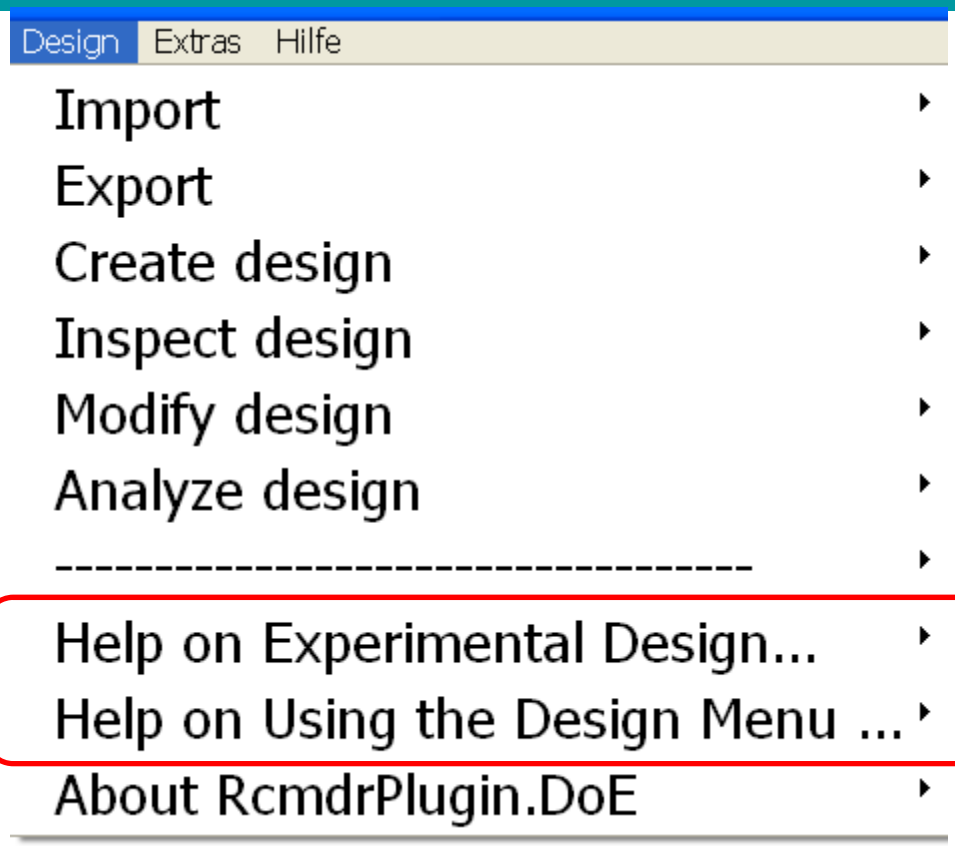
Store, load and reset dialog entries

RcmdrPlugin.DoE
plugin for ***R*** Commander (tcltk)

The GUI concept: Structure



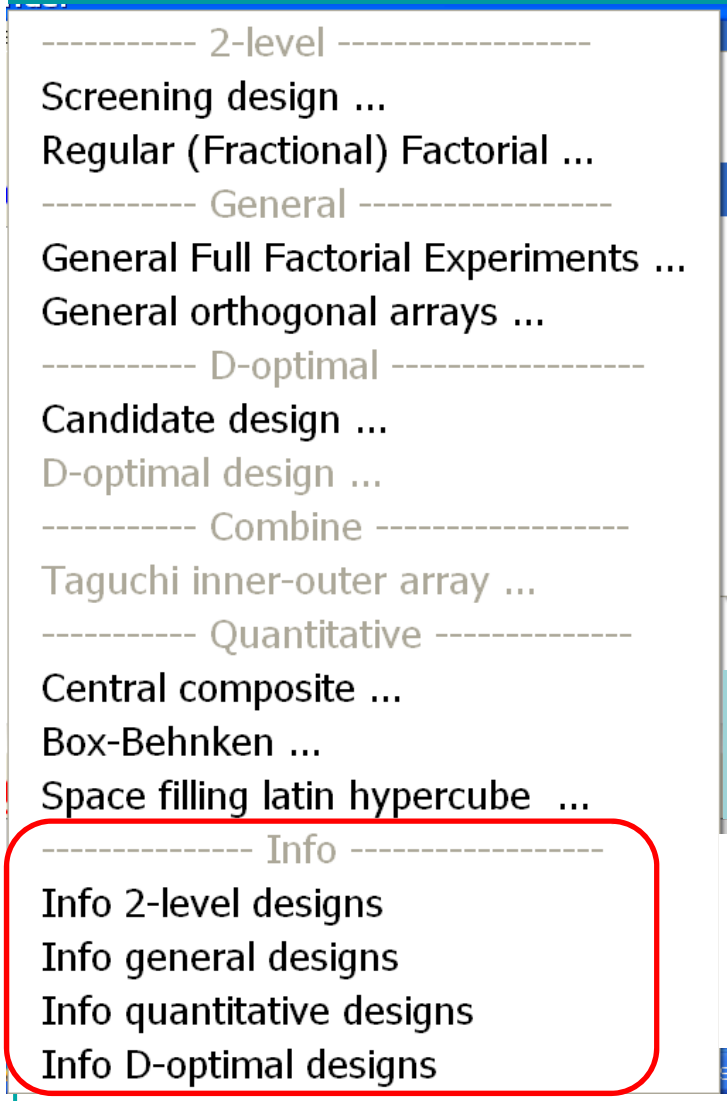
The GUI concept: guidance

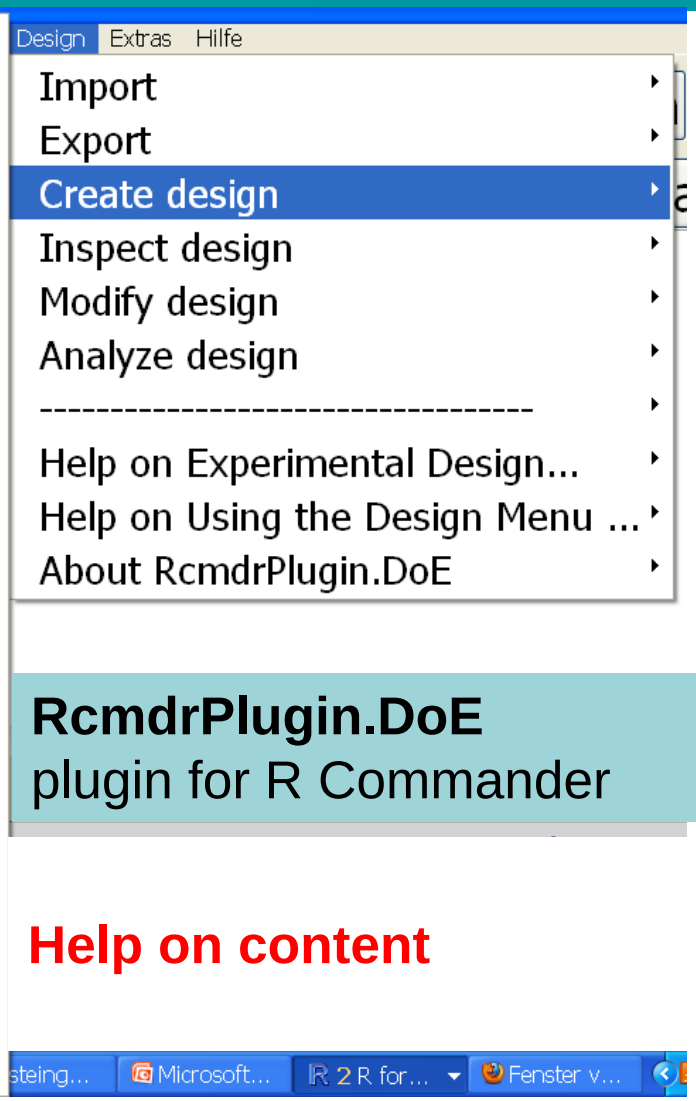


Help on content and help on usage

RcmdrPlugin.DoE
plugin for ***R*** Commander

The GUI concept: guidance





RcmdrPlugin.DoE
plugin for R Commander

Help on content

The GUI concept: guidance?

- Request for more firm guidance
  - Allegation: A system like this leaves too much freedom to naïve users, they will be lost in possibilities and make wrong choices.
  - Expert system like approach preferred (like, e.g., in Stavex™):
    lead users through
    (what the software designers feel is)
    the **one and only path** of
    - design definition
    - and analysis steps

Not my cup of tea,
but I can see where it comes from

- Desirable – but very work-intensive – solutions:
  - automated expert system option,
    i.e. users can request firm guidance (but don‘t have to)
  - flow charts with recommendations
  - guidance for specific application areas, like Six Sigma projects
  - ...

Call for activities

A lot is already there – it is worth while to be added to
→ make ***R*** cover a broader range of DoE facilities

- Do you have expertise in an area of DoE
  which is not yet covered well in ***R*** ?
  - Write a package, or contribute functionality to an existing package
  - Try to stay close to existing structures
  - Make running projects known in order to avoid redundant work
    - I consider creating a section in the task view
      that points to running projects

- Do you have solid knowledge about optimal DoE ?
  Do you have experience with C code within a package ?
  Willing to take over **AlgDesign** for optimal DoE ?
  Please contact Bob Wheeler !

Call for activities

- Specific call for activities around my project
  (please contact me for these or further ideas):
  - Automated random effects analysis for split-plot designs,
    e.g. *appropriate random effects models for split-plot designs*
  - guidance facilities for the GUI
  - Implementation of functionality into **DoE.wrapper** and/or **RcmdrPlugin.DoE** (e.g. **`mixDesign`** from package **qualityTools**)
  - SAS macro-like functionality (%MktEx, Kuhfeld 2010) for intricate (market research) designs based on orthogonal arrays (challenge!)

And of course:

- bug reports,
- suggestions for improvement,
- wishes,
- beta-testing for **RcmdrPlugin.DoE**,
- internationalization (not quite yet)
- ...

References

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Passenger seat picture

Mike Babb (2005). Inside of a DeLorean DMC-12 Automobile. The Quintessential DeLorean Website www.babbtechnology.com (German Wikipedia “Autositze”).

References

References

CRAN R-packages not in the Experimental Design Task View

- **igraph:** Network analysis and visualization; *Gabor Csardi*
- **Rcmdr:** R Commander; *John Fox* with contributions from many others
- **relimp:** Relative Contribution of Effects in a Regression Model; David Firth with contributions from Heather Turner
- **scatterplot3d:** 3D Scatter Plot; *Uwe Ligges*
- **sfsmisc:** Utilities from Seminar fuer Statistik ETH Zürich; *Martin Mächler and many others*
- **SPOT:** Sequential Parameter Optimization; T. Bartz-Beielstein with contributions from: J. Ziegenhirt, W. Konen, O. Flasch, P. Koch, M. Zaefferer
- **vcd:** Visualizing Categorical Data; David Meyer, Achim Zeileis and Kurt Hornik, with contributions from Michael Friendly

Commercial software

- ***Stavex™***, AICOS Technologies AG
- **%MktEx macros (Kuhfeld 2010) running in *SAS*® software, by SAS Institute Inc.**