

## CRAN Task View: Design of Experiments (DoE) & Analysis of Experimental Data

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This task view collects information on R packages for experimental design and analysis of data from experiments. With a strong increase in the number of relevant packages, packages that focus on analysis only and do not make relevant contributions for design creation are no longer added to this task view. Please feel free to suggest enhancements, and please send information on new packages or major package updates if you think they belong here. Contact details are given on my [Web page](#).

Experimental design is applied in many areas, and methods have been tailored to the needs of various fields. This task view starts out with a section on the historically earliest application area, agricultural experimentation. Subsequently, it covers the most general packages, continues with specific sections on industrial experimentation, computer experiments, and experimentation in the clinical trials contexts (this section is going to be removed eventually; experimental design packages for clinical trials will be integrated into the clinical trials task view), and closes with a section on various special experimental design packages that have been developed for other specific purposes. Of course, the division into fields is not always clear-cut, and some packages from the more specialized sections can also be applied in general contexts. You may also notice that my own experience is mainly from industrial experimentation (in a broad sense), which may explain a somewhat biased view on things.

### Experimental designs for agricultural and plant breeding experiments

Package [agricolae](#) is by far the most-used package from this task view (status: October 2017). It offers extensive functionality on experimental design especially for agricultural and plant breeding experiments, which can also be useful for other purposes. It supports *planning* of lattice designs, factorial designs, randomized complete block designs, completely randomized designs, (Graeco-)Latin square designs, balanced incomplete block designs and alpha designs. There are also various *analysis* facilities for experimental data, e.g. treatment comparison procedures and several non-parametric tests, but also some quite specialized possibilities for specific types of experiments. Package [desplot](#) is made for plotting the layout of agricultural experiments. Package [agridat](#) offers a large repository of useful agricultural data sets.

### Experimental designs for general purposes

There are a few packages for creating and analyzing experimental designs for general purposes: First of all, the standard (generalized) linear model functions in the base package stats are of course very important for analyzing data from designed experiments (especially functions `lm()`, `aov()` and the methods and functions for the resulting linear model objects). These are concisely explained in Kuhnert and Venables (2005, p. 109 ff.); Vikneswaran (2005) points out specific usages for experimental design (using function `contrasts()`, multiple comparison functions and some convenience functions like `model.tables()`, `replications()` and `plot.design()`). Lawson (2014) is a good introductory textbook on experimental design in R, which gives many example applications. Lalanne (2012) provides an R companion to the well-known book by Montgomery (2005); he so far covers approximately the first ten chapters; he does not include R's design generation facilities, but mainly discusses the analysis of existing designs. Package [GAD](#) handles general balanced analysis of variance models with fixed and/or random effects and also nested effects (the latter can only be random); they quote Underwood (1997) for this work. The package is quite valuable, as many users have difficulties with using the R packages for handling random or mixed effects. Package [granova](#) offers some interesting non-standard graphical representations for results of simply-structured experiments (one-way and two-way layouts, paired data), package [ez](#) aims at supporting intuitive analysis and visualization of factorial experiments based on package "ggplot2".

- Package [AlgDesign](#) creates full factorial designs with or without additional quantitative variables, creates mixture designs (i.e., designs where the levels of factors sum to 1=100%; lattice designs are created only) and creates D-, A-, or I-optimal designs exactly or approximately, possibly with blocking, using the Federov (1972) algorithm.
- Package [skpr](#) also provides optimal designs (D, I, A, Alias, G, T, or E optimal); a selection of the optimality criteria can also be used for the stepwise creation of split-plot designs. The package can also assess the power of designs and display diagnostic plots. At the moment (October 2017), the algorithms used are not yet documented.
- Package [OptimalDesign](#) likewise calculates unblocked D-, A-, or I-optimal designs (they use "IV-optimal" instead of "I-optimal") exactly or approximately, treating quantitative variables only, including mixture designs; this package uses different algorithms (e.g. Atkinson, Donev and Tobias 2007, Harman and Filova 2014), some of which rely on the availability of the gurobi software ( <http://www.gurobi.com/>, free for academics and academic institutions) and its accompanying R package "gurobi" (not on CRAN).
- Package [ICAOD](#) implements the "Imperialist Competitive Algorithm for Optimal Designs" for nonlinear models according to Masoudi, Holling and Wong (2016). Package [LDOD](#) implements locally D-optimal designs for some nonlinear and generalized linear models, package [designGLMM](#) locally optimal designs for completely randomized or blocked Poisson models and package [PopED](#) provides optimal designs for nonlinear mixed effect models.
- There are various further packages that deal with optimal designs of different types: Package [rodd](#) provides T-optimal designs, also called optimal discriminating designs (Dette, Melas and Shpilev 2013, Dette, Melas and Guchenko 2014), Package [acebayes](#) calculates optimal Bayesian designs using an approximate coordinate exchange algorithm, package [OBsMD](#) provides "Objective Bayesian Model Discrimination in Follow-Up Designs" according to Consonni and Deldossi (2015). Further optimal design packages for very specific purposes are listed at the end of this view.
- Package [conf.design](#) allows to create a design with certain interaction effects confounded with blocks (function `conf.design()`) and allows to combine existing designs in several ways (e.g., useful for Taguchi's inner and outer array designs in industrial experimentation).
- Package [planor](#) allows to generate regular fractional factorial designs with fixed and mixed levels and quite flexible randomization structures. The packages flexibility comes at the price of a certain complexity and - for larger designs - high computing time.
- Package [ibd](#) creates and analyses incomplete block designs. Packages [PGM2](#), [RPPairwiseDesign](#) and [CombinS](#) all produce designs related to (resolvable) (partially) balanced incomplete block designs. Package [PBIBD](#) also provides experts with some series of partially balanced incomplete block designs.
- Package [crossdes](#) creates and analyses cross-over designs of various types (including latin squares, mutually orthogonal latin squares and Youden squares) that can for example be used in sensometrics. Package [Crossover](#) also provides crossover designs; it offers designs from the literature and algorithmic designs, makes use of the functionality in [crossdes](#) and in addition provides a GUI.
- Package [DoE.base](#) provides full factorial designs with or without blocking (function `fac.design`) and orthogonal arrays (function `oa.design`) for main effects experiments (those listed by Kuhfeld 2009 up to 144 runs, plus a few additional ones). There is also some functionality for assessing the quality of orthogonal arrays, related to Groemping and Xu (2014) and Groemping (2017), and some analysis functionality with half-normal effects plots in quite general form (Groemping 2015). Package [DoE.base](#) also forms the basis of a suite of related packages: together with [FrF2](#) (cf. below) and [DoE.wrapper](#), it provides the work horse of the GUI package [RcmdrPlugin.DoE](#) (beta version; tutorial available in Groemping 2011), which integrates design of experiments functionality into the R-Commander (package "Rcmdr", Fox 2005) for the benefit of those R users who cannot or do not want to do command line programming. The role of package [DoE.wrapper](#) in that suite is to wrap functionality from other packages into the input and output structure of the package suite (so far for response surface designs with package [rsm](#) (cf. also below), design of computer experiments with packages [lhs](#) and [DiceDesign](#) (cf. also below), and , and D-optimal designs with package [AlgDesign](#) (cf. also above).
- Package [DoE.MIParray](#) creates optimized orthogonal arrays (or even supersaturated arrays) for factorial experiments. Arrays created with this package can be used as input to function `oa.design` of package [DoE.base](#). Note, however, that the package is only useful in combination with at least one of the

commercial optimizers [Gurobi](#) (R-package `gurobi` delivered with the software) or [Mosek](#) (R-package `Rmosek` downloadable from the vendor (an outdated version is on CRAN)).

- Package [dae](#) provides various utility functions around experimental design and R factors, e.g. a randomization routine that can handle various nested structures (according to Bailey 1981) and functions for combining several factors into one or dividing one factor into several factors. Furthermore, the package provides features for post-processing objects returned by the `aov()` function, e.g. extraction of Yates effects for 2-level experiments.
- Package [daewr](#) accompanies the book *Design and Analysis of Experiments with R* by Lawson (2014) and does not only provide data sets from the book but also some standalone functionality that is not available elsewhere in R, e.g. definitive screening designs.
- Package [OPDOE](#) accompanies the book *Optimal Experimental Design with R* by Rasch et al. (2011). It has some interesting sample size estimation functionality, but is almost unusable without the book (the first edition of which I would not recommend buying).
- Package [blockTools](#) assigns units to blocks in order to end up with homogeneous sets of blocks in case of too small block sizes; package [blocksdesign](#) permits the creation of nested block structures.
- There are several packages for determining sample sizes in experimental contexts, some of them quite general, others very specialized. All of these are mentioned here: packages [powerAnalysis](#), [powerbydesign](#) and [easypower](#) deal with estimating the power, sample size and/or effect size for factorial experiments. Package [JMdesign](#) deals with the power for the special situation of jointly modeling longitudinal and survival data, package [PwrGSD](#) with the power for group sequential designs, package [powerGWASinteraction](#) with the power for interactions in genome wide association studies, package [ssizeRNA](#) with sample size for RNA sequencing experiments, and package [ssize.fdr](#) for sample sizes in microarray experiments (requesting a certain power while limiting the false discovery rate).

## Experimental designs for industrial experiments

Some further packages especially handle designs for industrial experiments that are often highly fractionated, intentionally confounded and have few extra degrees of freedom for error.

Fractional factorial 2-level designs are particularly important in industrial experimentation.

- Package [FrF2](#) (Groemping 2014) is the most comprehensive R package for their creation. It generates regular Fractional Factorial designs for factors with 2 levels as well as Plackett-Burman type screening designs. Regular fractional factorials default to maximum resolution minimum aberration designs and can be customized in various ways, supported by an incorporated catalogue of designs (including the designs catalogued by Chen, Sun and Wu 1993, and further larger designs catalogued in Block and Mee 2005 and Xu 2009; the additional package [FrF2.catlg128](#) provides a very large complete catalogue for resolution IV 128 run designs with up to 23 factors for special purposes). Analysis-wise, [FrF2](#) provides simple graphical analysis tools (normal and half-normal effects plots (modified from [BsMD](#), cf. below), main effects plots and interaction plot matrices similar to those in Minitab software, and a cube plot for the combinations of three factors). It can also show the alias structure for regular fractional factorials of 2-level factors, regardless whether they have been created with the package or not. Fractional factorial 2-level plans can also be created by other R packages, namely [BHH2](#) and [qualityTools](#) (but do not use function `pbDesign` from version 1.54 of that package!), or with a little bit more complication by packages [conf.design](#), [planor](#) or [AlgDesign](#). Package [ALTopt](#) provides optimal designs for accelerated life testing.
- Package [BHH2](#) accompanies the 2nd edition of the book by Box, Hunter and Hunter and provides various of its data sets. It can generate full and fractional factorial two-level-designs from a number of factors and a list of defining relations (function `ffDesMatrix()`, less comfortable than package `FrF2`). It also provides several functions for analyzing data from 2-level factorial experiments: The function `anovaPlot` assesses effect sizes relative to residuals, and the function `lambdaPlot()` assesses the effect of Box-Cox transformations on statistical significance of effects.
- [BsMD](#) provides Bayesian charts as proposed by Box and Meyer (1986) as well as effects plots (normal, half-normal and Lenth) for assessing which effects are active in a fractional factorial experiment with 2-

level factors; package [OBsMD](#) provides the functionality for follow-up experiments for resolving ambiguities after applying the Bayesian analysis of package [BsMD](#).

- Package [unrep](#) provides a battery of methods for the assessment of effect estimates from unreplicated factorial experiments, including many of the effects plots also present in other packages, but also further possibilities.
- The small package [FMC](#) provides factorial designs with minimal number of level changes; the package does not take any measures to account for the statistical implications this may imply. Thus, using this package must be considered very risky for many experimental situations, because in many experiments some variability is caused by level changes. For such situations (and they are the rule rather than the exception), minimizing the level changes without taking precautions in the analysis will yield misleading results.
- Package [pid](#) accompanies an online book by Dunn (2010-2016) and also makes heavy use of the Box, Hunter and Hunter book; it provides various data sets, which are mostly from fractional factorial 2-level designs.

Apart from tools for planning and analysing factorial designs, R also offers support for response surface optimization for quantitative factors (cf. e.g. Myers and Montgomery 1995):

- Package [rsm](#) supports sequential optimization with first order and second order response surface models (central composite or Box-Behnken designs), offering optimization approaches like steepest ascent and visualization of the response function for linear model objects. Also, coding for response surface investigations is facilitated.
- Package [DoE.wrapper](#) enhances design creation from package [rsm](#) with the possibilities of automatically choosing the cube portion of central composite designs and of augmenting an existing (fractional) factorial 2-level design with a star portion.
- The small package [rsurface](#) provides rotatable central composite designs for which the user specifies the minimum and maximum of the experimental variables instead of the corner points of the cube.
- The small package [minimalRSD](#) provides central composite and Box-Behnken designs with minimal number of level changes; the package does not take any measures to account for the statistical implications this may imply. Thus, using this package must be considered very risky for many experimental situations, because in many experiments some variability is caused by level changes. For such situations (and they are the rule rather than the exception), minimizing the level changes without taking precautions in the analysis will yield misleading results.
- Package [OptimaRegion](#) provides functionality for inspecting the optimal region of a response surface for quadratic polynomials and thin-plate spline models and can compute a confidence interval for the distance between two optima.
- Package [Vdgraph](#) implements a variance dispersion graph (Vining 1993) for response surface designs created by package [rsm](#). Packages [VdgRsm](#) and [vdg](#) provide similar functionality with more variety.
- Package [qualityTools](#) can also create central composite designs and can visualize response surfaces.
- Package [EngrExpt](#) provides a collection of data sets from the book *Introductory Statistics for Engineering Experimentation* by Nelson, Coffin and Copeland (2003).

In some industries, mixtures of ingredients are important; these require special designs, because the quantitative factors have a fixed total. Mixture designs are handled by packages [AlgDesign](#) (function `gen.mixture`, lattice designs), [qualityTools](#) (function `mixDesign`, lattice designs and simplex centroid designs), and [mixexp](#) (several small functions for simplex centroid, simplex lattice and extreme vertices designs as well as for plotting).

Occasionally, supersaturated designs can be useful. The two small packages [mkssd](#) and [mxkssd](#) provide fixed level and mixed level k-circulant supersaturated designs. The aforementioned package [DoE.MIParray](#) can also provide (small!) supersaturated arrays (by choosing resolution II), but requires the presence of at least one of the commercial optimizers [Gurobi](#) or [Mosek](#).

## Experimental designs for computer experiments



Computer experiments with quantitative factors require special types of experimental designs: it is often possible to include many different levels of the factors, and replication will usually not be beneficial. Also, the experimental region is often too large to assume that a linear or quadratic model adequately represents the phenomenon under investigation. Consequently, it is desirable to fill the experimental space with points as well as possible (space-filling designs) in such a way that each run provides additional information even if some factors turn out to be irrelevant. The [lhs](#) package provides latin hypercube designs for this purpose. Furthermore, the package provides ways to analyse such computer experiments with emphasis on what follow-up experiments to conduct. Another package with similar orientation is the [DiceDesign](#) package, which adds further ways to construct space-filling designs and some measures to assess the quality of designs for computer experiments. The package [DiceKriging](#) provides the kriging methodology which is often used for creating meta models from computer experiments, the package [DiceEval](#) creates and evaluates meta models (among others Kriging ones), and the package [DiceView](#) provides facilities for viewing sections of multidimensional meta models.

Package [MaxPro](#) provides maximum projection designs as introduced by Joseph, Gul and Ba(2015). Package [SLHD](#) provides optimal sliced latin hypercube designs according to Ba et al. (2015), package [sFFLHD](#) provides sliced full factorial-based latin hypercube designs according to Duan et al. (2017). Package [simrel](#) allows creation of designs for computer experiments according to the Multi-level binary replacement (MBR) strategy by Martens et al. (2010). Package [minimaxdesign](#) provides minimax designs and minimax projection designs according to Mak and Joseph (2016).

Package [tgp](#) is another package dedicated to planning and analysing computer experiments. Here, emphasis is on Bayesian methods. The package can for example be used with various kinds of (surrogate) models for sequential optimization, e.g. with an expected improvement criterion for optimizing a noisy blackbox target function. Packages [plgp](#) and [dynaTree](#) enhance the functionality offered by [tgp](#) with particle learning facilities and learning for dynamic regression trees.

Package [BatchExperiments](#) is also designed for computer experiments, in this case specifically for experiments with algorithms to be run under different scenarios. The package is described in a technical report by Bischl et al. (2012).

## Experimental designs for clinical trials

This task view only covers specific design of experiments packages (which will eventually also be removed here); there may be some grey areas. Please, also consult the [ClinicalTrials](#) task view.

- Package [experiment](#) contains tools for clinical experiments, e.g., a randomization tool, and it provides a few special analysis options for clinical trials.
- Package [ThreeArmedTrials](#) provides design and analysis tools for three-armed superiority or non-inferiority trials. Beside the standard functionality, the package includes the negative Binomial response situation discussed in Muetze et al. (2016).
- Package [gsDesign](#) implements group sequential designs, package [GroupSeq](#) gives a GUI for probability spending in such designs, package [OptGS](#) near-optimal balanced group sequential designs. Package [gsbDesign](#) evaluates operating characteristics for group sequential Bayesian designs. Package [gset](#) handles group sequential equivalence testing. Package [seqDesign](#) handles group sequential two-stage treatment efficacy trials with time-to-event endpoints.
- Package [binseqtest](#) handles sequential single arm binary response trials.
- Package [asd](#) implements adaptive seamless designs (see e.g. Parsons et al. 2012).
- Package [OptInterim](#) is for two- and three-stage designs for longterm binary endpoints.
- Packages [bcrm](#) and [crmPack](#) offer Bayesian CRM designs.
- Package [MAMS](#) offers designs for multi-arm multi stage studies, [BayesMAMS](#) provides a Bayesian sample size calculations for these.
- Package [BOIN](#) provides Bayesian optimal interval designs, which are used in phase I clinical trials for finding the maximum tolerated dose.
- The [DoseFinding](#) package provides functions for the design and analysis of dose-finding experiments (for example pharmaceutical Phase II clinical trials); it combines the facilities of the "MCPMod" package

(maintenance discontinued; described in Bornkamp, Pinheiro and Bretz 2009) with a special type of optimal designs for dose finding situations (MED-optimal designs, or D-optimal designs, or a mixture of both; cf., Dette et al. 2008).

- Package [VNM](#) provides multi-objective optimal designs for simultaneously optimizing inference about the shape of the dose-response curve, ED50 and minimum effective dose (MED) for certain classes of logistic models.
- Package [TEQR](#) provides toxicity equivalence range designs (Blanchard and Longmate 2010) for phase I clinical trials, package [pipe.design](#) so-called *product of independent beta probabilities dose escalation* (PIPE) designs for phase I. Package [dfpk](#) implements a Bayesian dose-finding design using pharmacokinetics for phase I trials. Package [dferm](#) provides designs for classical or TITE continual reassessment trials in phase I.
- Packages [dfcomb](#) and [dfmta](#) provide phase I/II adaptive dose-finding designs for combination studies or single-agent molecularly targeted agent, respectively.
- Packages [ph2bayes](#) and [ph2bye](#) are concerned with Bayesian single arm phase II trials.
- Package [sp23design](#) claims to offer seamless integration of phase II to III.

## Experimental designs for special purposes

Various further packages handle special situations in experimental design:

- Package [desirability](#) provides ways to combine several target criteria into a desirability function in order to simplify multi-criteria analysis; desirabilities are also offered as part of package [qualityTools](#).
- [osDesign](#) designs studies nested in observational studies, [designmatch](#) can also be useful for this purpose.
- [qtlDesign](#) is for quantitative trait locus designs,
- [toxtestD](#) creates optimal designs for binary toxicity tests,
- [hiPOD](#) provides optimal designs for pooled next generation sequencing experiments,
- [designGG](#) creates optimal designs for genetical genomics experiments (see Li et al. 2009),
- packages [optbdmaeAT](#), [optrcdmaeAT](#) and [soptdmaeA](#) provide optimal block designs, optimal row-column designs, and sequential optimal or near-optimal block or row-column designs for two-colour cDNA microarray experiments, with optimality according to an A-, MV-, D- or E-criterion.
- Package [docopulae](#) implements optimal designs for copula models according to Perrone and Mueller (2016),
- [optDesignSlopeInt](#) provides an optimal design for the estimation of the ratio of slope to intercept, and
- Packages [edesign](#) and [MBHdesign](#) provide spatially balanced designs, allowing the inclusion of prespecified (legacy) sites. The more elaborate package [geospt](#) allows to optimize spatial networks of sampling points (see e.g. Santacruz, Rubiano and Melo 2014).
- Package [SensoMineR](#) contains special designs for sensometric studies, e.g., for the triangle test.
- Package [choiceDes](#) creates choice designs with emphasis on discrete choice models and MaxDiff functionality; it is based on optimal designs. Package [idefix](#) provides D-efficient designs for discrete choice experiments based on the multinomial logit model, and individually adapted designs for the mixed multinomial logit model (Crabbe et al. 2014). Package [support.CEs](#) provides tools for creating stated choice designs for market research investigations, based on orthogonal arrays.
- Package [odr](#) creates optimal designs for cluster randomized trials under condition- and unit-specific cost structures.
- Package [bioOED](#) offers sensitivity analysis and optimal design for microbial inactivation.

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