MSOpt	*MSOpt*

Description

The `MSOpt` function creates a list object containing the main information on the experiment settings and the optimization criteria to be considered. According to the declared criteria, it also provides the basic matrices for their implementation, such as moment matrices. `MSOpt` returns input objects of the `Score` and `MSSearch` functions of the multiDoE package.

Usage

```
MSOpt(facts, units, levels, etas, criteria, model)
```

Arguments

`facts` A list of vectors representing the distribution of factors across strata. Each item in the list represents a stratum and the first item is the highest stratum of the multi-stratum structure of the experiment. Within the vectors, experimental factors are indicated by progressive integer from 1 to the total number of experimental factors, starting from the highest strata. Blocking factors are denoted by empty vectors.

`units` A list containing the number of units in each stratum. For stratum i, the number of experimental units within each unit of the previous stratum (i-1) is indicated. `length(units)` must be equal to `length(facts)`.

`levels` A vector containing the number of available levels for each experimental factor (blocking factors are excluded). If all the experimental factors share the number of levels, one integer is sufficient.

`etas` A list specifying the ratios of error variance between subsequent strata. It follows that `length(etas)` must be equal to `length(facts) -1`.

`criteria` A list specifying the criteria to be optimized. It can contain any combination of:

- "I" : I-optimality
- "Id" : Id-optimality
- "D" : D-optimality
- "A" : Ds-optimality
- "Ds" : A-optimality
- "As" : As-optimality

More detailed information on the available criteria is given under 'Details'.

`model` A string which indicates the type of model, among "main", "interaction" and "quadratic".

Details

A little notation is introduced to present the criteria that can be used in the multi-objective approach of the multiDoE package.
For an experiment with N runs and s strata, with stratum i having n_i units within each unit

at previous stratum $(i-1)$ and stratum 0 being defined as the entire experiment $(n_0 = 1)$, the general form of the model can be written as:

$$y = X\beta + \sum_{i=1}^{s} Z_i \varepsilon_i$$

where y is a N-dimensional vector of responses $(N = \prod_{j=1}^{s} n_j)$, X is an $N \times p$ model matrix, β is a p-dimensional vector containing the p fixed model parameters, Z_i is an $N \times b_i$ indicator matrix of zero and ones for the units in stratum i and $b_i = \prod_{j=1}^{i} n_j$. Finally, the vector $\varepsilon_i \sim N(0, \sigma_i^2 I_{b_i})$ is a b_i-dimensional vector containing the random effects, which are all incorrelated. The variance components $\sigma_i^2 (i = 1, \ldots, s)$ have to be estimated and this is usually done by using the REML method. The best linear unbiased estimator for the parameter vector β is the generalized least square estimator:

$$\hat{\beta}_{GLS} = (X' * V^{-1} * X)^{-1} * X' * V^{-1} * y$$

. This estimator has variance-covariance matrix:

$$Var(\hat{\beta}_{GLS)=\sigma^2(X'V^{-1}X)^{-1}}$$

, where $V = \sum_{i=1}^{s} \eta_i Z_i' Z i$, $\eta_i = \frac{\sigma_i^2}{\sigma^2}$ and $\sigma^2 = \sigma_s^2$. The variance components $\sigma_i^2 (i = 1, \ldots, s)$ have to be estimated and this can be done by using the REML method. Finally, let $M = X'V^{-1}X$ be the information matrix of $\hat{\beta}$ when the GLS estimator is used to estimate model parameters in a multi-stratum experiment.

\item **D-optimality.** The D-optimality criterion is based on minimizing the generalized variance of the parameter estimates. This can be done either by minimizing the determinant of the variance-covariance matrix of $\hat{\beta}$ or by maximizing the determinant of M.
The objective function to be minimized is:

$$f_D(d; \eta) = \left(\frac{1}{\det(M)} \right)^{1/p}$$

, where d is the design with information matrix M and p is the number of model parameters.

\item **A-optimality.** This criterion is based on minimizing the average variance of the estimates of the regression coefficient. The sum of the variances of the parameter estimates (elements of $\hat{\beta}$) is taken as a measure, which is equivalent to the trace of M^{-1}.
The objective function to be minimized is:

$$f_A(d; \eta) = \mathtt{tr}(M^{-1})$$

, where d is the design with information matrix M

\item **I-optimality.** The I-optimality criterion seeks to minimize the average prediction variance. The objective function to be minimized is:

$$f_I(d; \eta) = \frac{\int_\chi f'(x)(X'V^{-1}X)^{-1} f(x)\, dx}{\int_\chi dx}$$

, where χ represents the design region.
When there are k treatment factors and the experimental region is $[-1, +1]^k$, the objective function can also be written as:

$$f_I(d; \eta) = \mathtt{tr}\left[(X'V^{-1}X)^{-1} B\right]$$

, where $B = 2^{-k} \int_\chi f'(x) f(x)\, dx$, is the moment matrix

\item **Id-optimality.** \item **As-optimality.** \item **Ds-optimality.**

Value

MSOpt returns a list containing the following components:

facts	The argument facts.
nfacts	An integer. The number of expermental factors (bloking factors are excluded from the count).
nstrat	An integer. The number of strata.
units	The argument units.
runs	An integer. The number of runs.
etas	The argument etas.
avlev	A list showing the available levels for each experimental factor.
levs	A vector showing the number of available levels for each experimental factor.
Vinv	The inverse of the variance-covariance matrix of the responses.
model	The argument model.
crit	The argument criteria.
ncrit	An integer. The number of criteria.
M	The moment matrix. Only with *I-optimality* criteria; .
M0	The moment matrix. Only with *Id-optimality* criteria.
W	The diagonal matrix of weights. Only with *As-optimality* criteria.

More information on M, M0 and W can be found in the descriptions of the respective criteria under 'Details'.