

CMAT Newsletter: July 2008, Part I

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1 General Remarks

Most of the time during this last half year I spent on the following problems:

1. Adding more complicate examples to the `tnlp` directory of the `nlp` function. This uncovered many bugs, mostly connected to some features of `nlp` but also some general language problems.
2. Extending the functionality of the MDS function.
3. Adding some basic statistics routines based on code by my former class mate Andreas Hahnewald-Busch from the TU Dresden.

During some work on my wifes Microchip data which contains some rather long string data including special symbols, tabs and spaces, I had to improve the printout for vectors and matrices. Now long strings can wrap around in columns of tables taking multiple lines.

One of class mates when I studied Math from 1966 until 1971 was Andreas Hahnewald-Busch. I met Andeas already before we studied at the TU Dresden in a French language class at the evening school *Volkshochschule* in Dresden. Even though Andreas choose *Probabilistic Statistics* as his special topic and I choose *Numerical Mathematics* we never lost touch until his tragic dead. When I was employed at the Academy of Sciences in Berlin I needed a computer in Dresden to develop my software and Andreas gave me permission to use his computer account on the BESM-6 computer of the TU Dresden. Later when I applied for emigration I made him to my successor in a well paid side job teaching Pharmacists in Math and Computer Science at a College in Dresden. When I had to emigrate, I ask'd him to keep a few valuable things for me which I was not able to move to the West. Already working at SAS in the US, I called him rather often and mailed him at his wish a selection of SAS Software Manuals. The first mailing was obviously stolen by the East German authorities, however, the second mailing arrived. From talking to him on the phone, he was planning to write some new statistics software which was not available in SAS at that time.

From Hungary Andreas mailed me some listings of my older computer programs to the US, which was rather dangerous. I would never have ask'd him for this since I felt not even comfortable to pack such things into my moving boxes.

In memory of Andreas I implemented all his functions from the V. Nollau and A. Hahnewald-Busch book *"Statistische Analysen"* (1975) with the set of `hb...` functions. Note, the book and the original Algol code are from Pre-SAS time, and not much statistics software was available at that time. Even though much is covered by the `reg`, `discrim`, `gmod`, and `anova` functions already and my idea of CMAT is not to replicate what other software is already doing better I think of enhancing this software if I'll find some time in the near future.

1.1 New Functions

The following new functions are implemented:

codapp implements an important applications of the complete orthogonal decomposition (COD) for the solution of rank-deficient linear least squares problems (similar to the APPCORT function which I put into SAS/IML many years ago; as the CMAT function cod is similar to the COMPORF function which I wrote for SAS/IML).

hbanova implements nine different versions of analysis of variance for models I and II (chapters 4 and 7, A4.3, A4.4)

hbaddtst test for additivity by Tukey (chapter 4.5, A4.2)

hbbartlett Bartlett test (chapter 4.4, A4.1)

hbscheffe Scheffè (1959) test (chapter 4.3, A4.5)

hbcovar one way classification with one covariable and unrepeated two way classification with one covariable (chapters 5.1 and 5.2, A5) (AHB did not implement the (2,2) model of chapter 5.3)

hbdiscrim two class discriminant analysis (chapter 6.1, A3) (AHB did not implement the N class analysis which is described in chapter 6.2)

hblreg linear regression (simple version of the **reg** function) (chapters 3.1 to 3.3, A2.2)

hbltst linearity test by R. A. Fisher (chapter 2.9, A2.1)

hbqlreg simple (one predictor) quasi linear polynomial regression (chapter 3.5, A2.3)

hbrcmp compare the coefficients of two simple linear regressions (chapter 3.3, A2.4)

mbs computes a variety of methods for *metric* and *nonmetric* multidimensional scaling (MDS) for 2-and 3-way data tables

selc sequential elimination of level combinations algorithm (JSS 317)

strquot reading data sets containing string data where strings are unquoted but separated by a specific separator string like a new line symbol

urd1out analysis of unreplicated 2^k and 2^{k-p} designs with a possible outlier

1.2 Fixed Bugs

By adding rather large examples for the `nlp` function, like those for neural nets, the efficient frontier of the Markowitz stock portfolio model, and some examples which I designed for an ASA meeting long time ago together with Ying So and Minbo Kim, the CMAT language was tested very extensively and still a large number of bugs were found. Some rather serious bugs were found not only in the `ode` and `nlp` functions, also in some more general language features.

The first time we dealt with long and non standard strings (containing special symbols and white space) in data describing genes. The `[` and `]` operators work only for standard strings (not containing white space or special symbols). A new function `strquot` was written recognizing a specific separator string (can be a new line) indicating the end of a string. Bugs had to be fixed also in printing functions for objects with oversize columns, i.e. long strings not fitting the specified line size.

2 Modifications of Features

2.1 Extensions to Various Functions

2.1.1 Extension of min and max Functions

$$z = \max(a,b)$$

$$z = \max(a)$$

$$z = \max(a,b,c,\dots)$$

Purpose: The arguments can be scalars or data objects like vectors, matrices, or tensors.

z=max(a,b) This is the common form:

- If one of the two arguments is scalar and the other argument is a matrix or vector, then the function is performed using the scalar and each entry of the other operand. The result is of the same size as the matrix or vector argument.
- If both arguments are vectors or matrices, then both must have the same dimension (same number of rows and columns). The function is performed pairwise with corresponding pairs of entries of the two operands.

For integer and real arguments the result is

$$z = \max(a, b) = \begin{cases} a & \text{if } a \geq b \\ b & \text{if } a < b \end{cases}$$

For complex arguments a or b the decision is based on the modulus (absolute values) of the arguments.

z=max(a) If **a** is an object, the largest nonmissing numerical entry of *a* is returned.

z=max(a,b,c,...) The arguments can be scalars or data objects not necessarily of the same size. The result *z* is the largest scalar entry of all arguments.

If the arguments have no nonmissing values (strings), a missing value is returned.

Input: The arguments *a* and *b* must be numeric scalars, vectors, matrices, or tensors.

Output: z=max(a,b) The result *z* is a scalar if both, *a* and *b* are scalars. Otherwise it is a data object of the same size as one or both of the arguments.

z=max(a) The result *z* is a scalar.

z=max(a,b,c,...) The result *z* is a scalar.

The data type of the result *z* is the same as the maximum data type of all arguments in the order integer, real, complex. For complex arguments *a* or *b* the returned value is complex, either *a* or *b*, however the pairwise comparison is based on their modulus (the absolute values).

- Restrictions:**
1. Missing value is returned if arguments contain string data or missing values.
 2. For $z = \max(a,b)$ and if *a* or *b* is an object then the other argument must be either scalar or an object of the same size.

Relationships: min()

Examples: 1. Example for 2-argument form max(a,b):

```
a = [ 3., -3., 2., -2. ];
b = [ -1., 1., -3., 3. ];
d = min(a,b);
print "Min=", d;
e = max(a,b);
print "Max=", e;
```

Min=		1	Max=		1
-----			-----		
1	-1.00000		1	3.00000	
2	-3.00000		2	1.00000	
3	-3.00000		3	2.00000	
4	-2.00000		4	3.00000	

2. Example for 1-argument form `max(a)`:

```
q = [ 0. 1. 1. 3. 5. -3. ];  
print "Min=", qmin = min(q);  
print "Max=", qmax = max(q);
```

```
Min=-3.0000  
Max= 5.0000
```

3. Example for more than two argument form `max(a,b,c,...)`:

```
a = [ 1 2 3 ]; b = [ 3 4 , 5 6 ]; c = 7.;  
print "Min=", d = min(a,b,c);  
print "Max=", e = max(a,b,c);
```

```
Min= 1  
Max= 7
```

```
z = min(a,b)  
z = min(a)  
z = min(a,b,c,...)
```

Purpose: The arguments can be scalars or data objects like vectors, matrices, or tensors.

z=min(a,b) This is the common form:

- If one of the two arguments is scalar and the other argument is a matrix or vector, then the function is performed using the scalar and each entry of the other operand. The result is of the same size as the matrix or vector argument.
- If both arguments are vectors or matrices, then both must have the same dimension (same number of rows and columns). The function is performed pairwise with corresponding pairs of entries of the two operands.

For integer and real argument the result is

$$z = \min(a, b) = \begin{cases} a & \text{if } a \leq b \\ b & \text{if } a > b \end{cases}$$

For complex arguments a or b the decision is based on the modulus (absolute values) of the arguments.

z=min(a) If a is an object, the smallest nonmissing numerical entry of a is returned.

z=min(a,b,c,...) The arguments can be scalars or data objects not necessarily of the same size. The result z is the smallest scalar entry of all arguments.

If the arguments have no nonmissing values (strings), a missing value is returned.

Input: The arguments a and b must be numeric scalars, vectors, matrices, or tensors.

Output: z=min(a,b) The result z is a scalar if both, a and b are scalars. Otherwise it is a data object of the same size as one or both of the arguments.

z=min(a) The result z is a scalar.

z=min(a,b,c,...) The result z is a scalar.

The data type of the result z is the same as the maximum data type of all arguments in the order integer, real, complex. For complex arguments a or b the returned value is complex, either a or b , however the pairwise comparison is based on their modulus (the absolute values).

Restrictions: 1. Missing value is returned if arguments contain string data or missing values.

2. For $z = \min(a,b)$ and if a or b is an object then the other argument must be either scalar or an object of the same size.

Relationships: `max()`

Examples: 1. Example for 2-argument form `max(a,b)`:

```
a = [ 3., -3., 2., -2. ];
b = [ -1., 1., -3., 3. ];
d = min(a,b);
print "Min=", d;
e = max(a,b);
print "Max=", e;
```

Min=		1	Max=		1

1		-1.00000	1		3.00000
2		-3.00000	2		1.00000
3		-3.00000	3		2.00000
4		-2.00000	4		3.00000

2. Example for 1-argument form `max(a)`:

```

q = [ 0. 1. 1. 3. 5. -3. ];
print "Min=", qmin = min(q);
print "Max=", qmax = max(q);

```

```

Min=-3.0000
Max= 5.0000

```

3. Example for more than two argument form `max(a,b,c,...)`:

```

a = [ 1 2 3 ]; b = [ 3 4 , 5 6 ]; c = 7.;
print "Min=", d = min(a,b,c);
print "Max=", e = max(a,b,c);

```

```

Min= 1
Max= 7

```

2.1.2 Extension of `irtml` Function

1. When the new "size" option is specified the data matrix can have an additional column specifying pattern probability values (normally $0 \leq p_i \leq 1$ and $\sum_i p_i = 1$). The sample size is then specified by "size" with an int or real scalar. The pattern of the input matrix must be distinct.
2. The *R1* goodness of fit measure is computed and returned when all items are dichotomous and the "nor1" option is not specified.

2.1.3 Extension of `cod` Function

The function for the complete orthogonal decomposition

`r = cod(a)` or `<q,r,v,pi> = cod(a)`

was extended for a second and third input argument to `r = cod(a,<b<sopt>>)` or `<q,r,v,pi,lind> = cod(a,<b<sopt>>)`.

If the second input argument `b` is specified other than missing, it must be a vector or matrix **B** having the same number of rows as the first argument `a`. If `b` is specified nonmissing, the result `q` returns $\mathbf{Q}^T \mathbf{B}$ rather than **Q**. This extension is useful for the major application of this function for solving rank deficient least squares problems, see also the new function `codapp()`.

The third input argument `sopt` is a string option specifying one of two algorithms.

"old" an older algorithm which was already available and should be used together with the LAPACK option.

"new" a newly developed algorithm.

At this time no sufficient test computations were made to determine which of the algorithms is the preferred one.

2.1.4 Extension of mds Function

The `mds` function was extended by features of the MULTISCALE algorithm by Jim Ramsay (1969, 1977). Those include:

- The spline transform among dissimilarity data and model distances.
- Three different model types for subjective weights:
 1. the identity model,
 2. the d diagonal weighting model, which includes the estimation of $nsub \times d$ weights.
 3. and the full $d \times d$ symmetric weighting matrix, which includes the estimation of $nsub \times d * (d + 1)/2$ weights.
- The computation of asymptotic standard errors for the point coordinates. (Not yet for the weight estimates.) This is implemented for four different data distribution assumptions:

- 1.

Asymptotic standard errors and confidence ellipsoids are at this time only for the unrotated point coordinates as with the MULTISCALE program.

Instead of listing here the additions to the function we prefer to give a complete new documentation of the function in the *New Developments* section below.

2.1.5 Extensions to ode Function

The old form of the `ode` call utilized a numeric vector for specifying a number of options. Now, the `optn` argument must be specified in form of a two column matrix where the first column defines the option as string value (in quotes) and the second column can be used for a numeric or string specification of the option.

```
y = ode(func,tab,y0<,optn<,root<,afun<,jacm>>>)
```

```
<y,t> = ode(func,tab,y0<,optn<,root<,afun<,jacm>>>)
```

All other features of the `ode` function are unchanged.

Option	Second Column	Meaning
"maxord"	int	maximum order of interpolation; by default: "maxord"=5 for Gear's method (i.e. "gear" or "dyna", and "maxord"=12 for Adams method (i.e. "adam") this option does not apply to methods "rk45" and "rk56"
"maxst"	int	maximum number of internal steps performed within any of the integration intervals; the default is "maxst"=1000
"met"	string "adam" "gear" "dyna" "rk45" "rk56"	integration method: stiff-nonstiff Adam's method: only for nonstiff ODE's Gear's method: also for stiff ODE's (default) method choosing dynamically between "adam" and "gear", (note, that "dyna" is not possible for "nroot" > 0) Fehlberg's (4,5) order Runge-Kutta (similar to Watts and Shampine) Verner's (5,6) order Runge-Kutta method (similar to an implementation by Jackson)
"minval"	real	specifies the smallest nonzero value for solution y_i ; the ODE function will not approximate exactly values for y_i smaller than "maxst"; default is 0. this option does not apply to methods "rk45" and "rk56"
"nequ"	int	only valid for "type"=2: specifies the number m of ODE's of the hybrid problem; default is "nequ"=n this option does not apply to methods "rk45" and "rk56"
"nolog"		supresses output of warnings into the log
"nroot"	int	number of roots t_r returned by user function $x=ROOT(i, t, y)$; the iteration is stopped when the first specified root $t_0 \leq t_r \leq t_N$ is reached; default is 0 this option does not apply to methods "rk45" and "rk56"
"print"	int 0 1 2	controls printed output 0 no printed output 1 print information at begin and end of iteration 2 print iteration history additionally

Option	Second Column	Meaning
"reltol"	real	relative precision of integration (def=1.e-4)
"task"	string	compute y values at t_1, \dots, t_N exactly or permit for interpolation; default is "task" = "int":
	"int"	for t[1] until t[N-1] interpolated (like "task" = "eff"), for t[N] precisely (like "task" = "exa")
	"eff"	interpolation is permitted for the y values at t_1, \dots, t_N
	"exa"	all t_1, \dots, t_N are matched precisely; this is computationally very expensive
"type"	int	which kind of problem is to be solved
	0	explicit initial value problem: $\frac{dy_i}{dt} = f_i(y, t), \quad i = 1, \dots, n$
	1	this is default implicit initial value problem: $\mathbf{A} \frac{dy}{dt} = f(y, t)$
	2	where function a=AFUN(t, y) must return return $n \times n$ matrix A for given t and n vector y hybrid system of m ODE's and $n - m$ algebraic equations $\begin{aligned} \mathbf{a}_i \frac{dy_i}{dt} &= f_i(y, t), \quad i = 1, \dots, m \\ 0 &= f_i(y, t), \quad i = m + 1, \dots, n \end{aligned}$
		where the user function a=AFUN(t, y) must return n vector a for given t and n vector y

2.1.6 Extensions to nlp and nle: New Returns

The following was the old syntax for calling **nle** and **nlp**:

```
< xr, rp > = nle(func, x0<, sopt<, par, <jac>>>)
```

```
< xr, rp > = nlp(func, x0<, keyopt<, lau<, lbub<, nlcon, <grad, <hess, <jcon>>>>>>>>>>>>)
```

We added some more return arguments to the two functions:

```
< xr, rp, der1 > = nle(func, x0<, sopt<, par, <jac>>>)
```

```
< xr, rp, der1, der2, acon, dpro, jhnlc > = nlp(func, x0<, keyopt<, lau<, . . . , <jcon>>>>>>>>>>>>)
```

The following results are returned only if available for the specific optimization technique:

der1 except for derivative free methods, **der1** contains in its first row the gra-

dient at the solution \mathbf{xr} . If an $m \times n$ Jacobian was used it is stored in rows 2, ..., $m + 1$.

der2 if the Hessian or cross-product Jacobian was used by the optimization technique, **der2** contains this $n \times n$ matrix evaluated at the solution \mathbf{xr} .

acon returns a column vector or a 3 or 5 column matrix indicating

1. in column 1: active boundary constraints
2. in column 2 and 3: values of linear constraints and which are active at the solution
3. in column 4 and 5: values of nonlinear constraints which are active at the solution

dpro contains only for constrained optimization: the vector of projected gradient in its first row and if available the projected Hessian matrix in additional rows.

jhnlc contains only for nonlinearly constrained optimization: either the Jacobian or the Hessian of the nonlinear constraints.

2.1.7 Extensions to nlp Function

Modifying the nlp Function: Some Options The default value for the **nlnrmit** option specifying the maximum number of preprocessor iterations for reducing the violation of nonlinear constraints at the starting point was set to zero (from former 10 iterations). Also constraints are no longer scaled by default, it must now be invoked by specifying the **cscale** option.

In a postprocessing step, the optimality of a solution may be tested by evaluating the function on points of a circle around the parameter estimate. The **rtop** option specifies a radius of the circle. Infeasible circle points are not evaluated.

Extensions to nlp Function: Grid Search Until now, the input argument **x0** for the starting point had to be a n vector. We now allow also the input of a $n \times k$ matrix where each row in its first $k_i, i = 1, \dots, n$ columns specifies grid points for an initial estimate. Usually, $k = \max_{i=1}^n k_i$. The remaining columns k_i, \dots, k of row i must be set to missing values. During a preprocessor step, all $\prod_{i=1}^n k_i$ starting points are evaluated and the best is selected for the starting point. Note, missing values and multiple grid values are removed from the grid. The new "**best**" option specifies an integer number of best points to be printed with their corresponding function values.

If there are constraints specified, the **nofea** option drops infeasible points from the grid evaluation.

```
function frosbr2(x) {
  f = cons(2);
  f[1] = 10. * (x[2] - x[1] * x[1]);
```

```

    f[2] = 1. - x[1];
    return(f);
}

x1 = [ -1.2  -5.:1.:9.  -2. ];
x2 = [ 1.:2.:5. 14#. ];
x0 = x1 |> x2; print "Grid=",x0;

/* Levenberg-Marquardt */
mopt = [ "tech"    "levmar" ,
         "pbest"      10 ,
         "print"      3 ];
< xr,rp,der1 > = nlp(frosbr2,x0,mopt);
print "LM LSQ: DER1=",der1;

```

Extensions to nlp Function: New Techniques Three additional conjugate gradient methods were added

”**bm**” spectral conjugate gradient method by Birgin & Martinez (2001) with restart as proposed by Andrei (2007)

”**spr**” scaled Polak-Ribière method (Andrei, 2007)

”**sfr**” scaled Fletcher-Reeves method (Andrei, 2007)

The three methods are implemented with two different restart methods which can be specified by the “**vers**” option:

0 performs angle restart testing the size of descent:

$$g_r^T d_r \geq -0.001 \|g_r\| \|d_r\|$$

1 performs Powell-Beale restart testing the orthonality of successive search directions:

$$\|g_r^T g_{r-1}\| \geq 0.2 \|g_r\|$$

2 performs restart as specified by the “**rest**” option specifying an integer number of iterations after which a restart is done.

The new methods are applied to the $n = 2$ Rosenbrock function:

```

real function frosbr1(x)
{
    /* crit = .5 * f' * f */
    s = 0.;

```

```

    r1 = 10. * (x[2] - x[1] * x[1]);
    r2 = 1. - x[1];
    crit = r1 * r1 + r2 * r2;
    return(crit);
}

real function grosbr(x)
{
    /* gradient= J' * f */
    f = cons(2);
    f[1] = 10. * (x[2] - x[1] * x[1]);
    f[2] = 1. - x[1];
    jacm = cons(2,2,1.);
    jacm[1,1] = -20. * x[1]; jacm[1,2] = 10.;
    jacm[2,1] = -1.;          jacm[2,2] = 0.;
    g = 2. * jacm' * f;
    return(g);
}

x0 = [ -1.2 1. ];

```

1. Compare the Birgin-Martinez method with our old Powell-Beale restart method:

```

print "Scaled Birgin-Martinez Procedure";
mopt = [ "tech" "congra" ,
         "upd"   "bm" ];
< xr, rp> = nlp(frosbr1,x0,mopt,,,,,grosbr);

```

Conjugate-Gradient Optimization
 Scaled Perry Update (Birgin & Martinez, 2001)
 Angle Restart
 User Specified Gradient

```

Iteration Start:
N. Variables          2
Criterion             24.20000000          Max Grad Entry  215.6000000

```

Iter	rest	nfun	act	optcrit	difcrit	maxgrad	alpha	slope
1	0	3	0	4.225209	19.97479	12.0012	8e-004	-54227.4
2	0	5	0	4.123315	0.101894	1.47559	1.23881	-0.16427

3	0	11	0	3.153859	0.969456	15.3256	366.441	-3e-003
4	0	13	0	2.935328	0.218531	18.1200	5e-003	-95.0228
5	0	14	0	1.939282	0.996047	1.97128	0.03898	-53.7121
6	0	16	0	1.651216	0.288065	5.72925	0.92313	-0.45306
7	0	18	0	1.504818	0.146398	8.83740	0.04532	-5.50434
8	0	19	0	1.047402	0.457416	2.06775	0.12171	-6.38630
9	0	23	0	0.533302	0.514099	5.50337	6.22620	-0.12101
10	0	24	0	0.242992	0.290310	5.45446	0.25691	-2.87669
11	0	26	0	0.172798	0.070195	0.76193	0.01766	-7.95091
12	0	29	0	0.107325	0.065473	3.19427	39.5250	-2e-003
13	0	30	0	0.059212	0.048114	4.13722	0.01550	-5.51292
14	0	32	0	0.038274	0.020937	0.49901	4e-003	-11.0304
15	0	35	0	0.017715	0.020559	2.07891	14.8899	-2e-003
16	0	36	0	3.6e-003	0.014159	1.39582	6e-003	-4.76617
17	0	38	0	2.6e-003	9.7e-004	0.19049	8e-004	-2.35155
18	0	41	0	2.7e-004	2.3e-003	0.53477	1.93390	-2e-003
19	0	43	0	4.9e-005	2.2e-004	0.05115	6e-004	-0.69930
20	0	45	0	4.8e-007	4.9e-005	0.02647	0.45229	-2e-004
21	0	47	0	1.2e-010	4.8e-007	1e-004	5e-004	-2e-003

Successful Termination After 21 Iterations
 ABSGCONV convergence criterion satisfied.
 Criterion 1.2240e-010 Max Grad Entry 0.000130196
 Slope SDirect. -0.002012364
 N. Function Calls 48 N. Gradient Calls 48
 Preproces. Time 0 Time for Method 1
 Effective Time 1

```
print "Powell-Beale Restart Procedure";
mopt = [ "tech" "congra" ,
        "upd"   "pb" ];
< xr, rp> = nlp(frosbr1,x0,mopt,,,,,grosbr);
```

Conjugate-Gradient Optimization
 Automatic Restart Update (Powell, 1977; Beale, 1972)
 User Specified Gradient

Iteration Start:
 N. Variables 2
 Criterion 24.20000000 Max Grad Entry 215.6000000

Iter	rest	nfun	act	optcrit	difcrit	maxgrad	alpha	slope
1	0	5	0	12.21263	11.98737	102.605	1e-003	-54227.4

2	1	9	0	4.465179	7.747455	31.8199	0.08022	-158.404
3	2	12	0	1.721788	2.743390	7.51549	4e-003	-1652.33
4	3	14	0	1.261716	0.460073	5.14185	0.04001	-17.1437
5	4	18	0	1.225464	0.036251	8.25795	3e-003	-25.8111
6	5	20	0	0.811041	0.414424	5.04328	0.01000	-68.4931
7	5	22	0	0.750370	0.060671	7.06388	0.02346	-4.41542
8	6	24	0	0.460088	0.290282	1.56525	0.01000	-52.9473
9	6	29	0	0.205633	0.254455	5.67494	0.28754	-1.36086
10	7	32	0	0.156114	0.049519	6.44849	3e-003	-24.1788
11	7	35	0	0.153919	2.2e-003	7.55008	1e-003	-7.63691
12	8	38	0	0.067512	0.086407	5.88641	4e-003	-84.5981
13	9	43	0	0.015795	0.051717	3.39118	4e-003	-20.6174
14	10	46	0	0.013784	2.0e-003	3.66717	1e-003	-3.22118
15	11	49	0	2.9e-003	0.010924	0.53580	1e-003	-17.8777
16	12	53	0	3.4e-004	2.5e-003	0.35287	0.02593	-0.15384
17	12	56	0	3.3e-004	1.3e-005	0.55227	2e-003	-0.04146
18	13	59	0	4.7e-005	2.8e-004	0.11433	3e-003	-0.33638
19	14	62	0	3.8e-005	8.4e-006	4e-003	1e-003	-0.01702
20	14	64	0	1.3e-005	2.5e-005	0.12006	0.25028	-2e-004
21	14	67	0	5.9e-006	7.2e-006	0.09242	1e-003	-0.01590
22	15	70	0	3.9e-008	5.8e-006	3e-003	1e-003	-0.01098
23	15	72	0	3.8e-008	8.7e-010	2e-003	0.11041	-2e-008
24	16	74	0	3.0e-013	3.8e-008	8e-006	0.02064	-4e-006

```

Successful Termination After      24 Iterations
ABSGCONV convergence criterion satisfied.
Criterion          3.0413e-013          Max Grad Entry  8.0078e-006
Slope SDirect.   -3.6728e-006
N. Function Calls          75          N. Gradient Calls          36
N. Line Searches          24          Preproces. Time            0
Time for Method           0          Effective Time             0

```

2. Compare the scaled Polak-Ribiere method with our old method:

```

print "Scaled Polak-Ribiere Procedure";
mopt = [ "tech" "congra" ,
        "upd"   "spr" ];
/* options debug="nlpcog*=4"; */
< xr, rp > = nlp(frosbr1,x0,mopt,.,.,.,grosbr);

```

Conjugate-Gradient Optimization

Scaled Polak & Ribiere Update (Birgin & Martinez, 2001)
 Angle Restart
 User Specified Gradient

Iteration Start:

N. Variables 2
 Criterion 24.20000000 Max Grad Entry 215.6000000

Iter	rest	nfun	act	optcrit	difcrit	maxgrad	alpha	slope
1	0	3	0	4.225209	19.97479	12.0012	8e-004	-54227.4
2	1	5	0	4.123326	0.101883	1.47590	1.23607	-0.16461
3	1	11	0	3.398703	0.724623	16.6396	295.210	-3e-003
4	1	13	0	3.148488	0.250214	19.5048	4e-003	-101.613
5	1	14	0	2.194519	0.953969	3.67853	0.02960	-70.6406
6	1	16	0	2.000833	0.193686	6.31449	0.33425	-1.02907
7	1	18	0	1.968548	0.032285	7.82874	0.02153	-2.79197
8	1	21	0	1.530584	0.437964	9.44477	0.12103	-6.78695
9	1	23	0	1.229539	0.301046	1.87472	0.08012	-7.74129
10	1	25	0	0.995246	0.234292	7.40442	12.3664	-0.03376
11	1	27	0	0.987355	7.9e-003	8.53973	0.01906	-0.95770
12	1	29	0	0.748566	0.238789	2.06697	0.17265	-2.83409
13	1	31	0	0.581345	0.167221	5.46329	5.19952	-0.05272
14	1	33	0	0.562095	0.019250	6.86845	0.03178	-1.18031
15	1	34	0	0.418152	0.143943	1.62207	0.05961	-3.65117
16	2	36	0	0.410735	7.4e-003	1.35378	0.32197	-0.04607
17	2	39	0	0.289956	0.120779	4.32608	18.3293	-0.01033
18	2	41	0	0.256048	0.033907	5.49160	0.01997	-3.10424
19	2	42	0	0.169400	0.086648	4.26835	0.02998	-9.01681
20	2	46	0	0.033225	0.136175	1.58459	0.59975	-0.15382
21	2	47	0	0.015496	0.017729	4.94562	0.02157	-5.09254
22	2	49	0	1.4e-003	0.014068	0.26340	5e-004	-59.8030
23	3	51	0	1.4e-003	3.7e-005	0.03097	4e-003	-0.02008
24	3	53	0	1.8e-004	1.2e-003	0.53704	2713.69	-1e-006
25	3	55	0	4.1e-005	1.4e-004	0.10794	5e-004	-0.54580
26	3	57	0	1.0e-005	3.0e-005	0.07347	7e-003	-8e-003
27	3	58	0	1.9e-007	1.0e-005	2e-003	4e-003	-5e-003
28	4	60	0	1.9e-007	2.2e-009	4e-004	6e-004	-8e-006

Successful Termination After 28 Iterations

ABSGCONV convergence criterion satisfied.

Criterion	1.8798e-007	Max Grad Entry	0.000379533
Slope SDirect.	-7.9765e-006		
N. Function Calls	61	N. Gradient Calls	61
Preproces. Time	0	Time for Method	0

Effective Time 0

```
print "UNscaled Polak-Ribiere Procedure";
mopt = [ "tech" "congra" ,
        "upd"   "pr"   ];
< xr, rp > = nlp(frosbr1,x0,mopt,.,.,.,, grosbr);
```

Conjugate-Gradient Optimization
Polak & Ribiere Update (Fletcher, 1980, 4.1.12)
User Specified Gradient

Iteration Start:

N. Variables 2
Criterion 24.20000000 Max Grad Entry 215.6000000

Iter	rest	nfun	act	optcrit	difcrit	maxgrad	alpha	slope
1	0	4	0	16.80653	7.393470	123.995	2e-003	-54227.4
2	1	9	0	6.986146	9.820384	74.6509	2e-003	-20689.4
3	2	13	0	4.230184	2.755962	15.2832	1e-003	-6631.44
4	3	17	0	4.065223	0.164961	1.83761	1e-003	-326.639
5	3	21	0	3.430994	0.634229	17.3148	0.28126	-3.07935
6	3	25	0	3.181065	0.249929	20.3821	1e-003	-347.942
7	3	30	0	1.399645	1.781420	4.06284	1e-002	-566.262
8	3	33	0	1.381114	0.018531	2.77742	2e-003	-24.2291
9	3	37	0	0.989928	0.391186	6.02301	0.05952	-9.44289
10	3	40	0	0.825493	0.164434	12.6224	0.02400	-36.8003
11	3	45	0	0.815083	0.010410	12.9909	7e-004	-31.0781
12	3	47	0	0.517657	0.297426	5.87687	5e-003	-239.950
13	4	50	0	0.433281	0.084376	3.81449	5e-003	-63.1391
14	5	53	0	0.410084	0.023197	2.10443	5e-003	-16.9923
15	6	56	0	0.399479	0.010605	1.54651	5e-003	-5.73771
16	6	59	0	0.386033	0.013446	4.51900	0.03124	-1.32944
17	6	62	0	0.272963	0.113070	10.5626	0.02400	-21.4661
18	6	64	0	0.121671	0.151292	10.4183	5e-003	-86.3239
19	6	67	0	0.029634	0.092037	1.49443	1e-003	-149.357
20	7	71	0	0.027814	1.8e-003	0.15268	1e-003	-2.71767
21	7	75	0	0.012246	0.015568	2.01672	0.83495	-0.02958
22	7	77	0	4.8e-004	0.011766	0.40836	5e-003	-5.67809
23	7	80	0	2.2e-004	2.6e-004	0.14575	1e-003	-0.31798
24	7	82	0	1.5e-004	7.0e-005	0.43475	5e-003	-0.04037
25	7	85	0	9.4e-005	6.0e-005	0.38651	8e-004	-0.16030
26	7	88	0	1.0e-007	9.4e-005	6e-003	1e-003	-0.18617

27	7	91	0	3.7e-008	6.6e-008	6e-003	0.02500	-9e-006
28	7	94	0	1.2e-008	2.4e-008	9e-005	1e-003	-5e-005

```

Successful Termination After      28 Iterations
ABSGCONV convergence criterion satisfied.
Criterion      1.2493e-008      Max Grad Entry  8.6491e-005
Slope SDirect. -4.9026e-005
N. Function Calls      95      N. Gradient Calls      51
N. Line Searches      28      Preproces. Time      0
Time for Method      0      Effective Time      0

```

3. Compare the scaled Fletcher-Reeves method with our old method:

```

print "Scaled Fletcher-Reeves Procedure";
mopt = [ "tech" "congra" ,
        "upd"   "sfr"  ];
< xr, rp> = nlp(frosbr1,x0,mopt,,,,,grobr);

```

```

                Conjugate-Gradient Optimization
Scaled Fletcher & Reeves Update (Birgin & Martinez, 2001)
                Angle Restart
                User Specified Gradient

```

```

Iteration Start:
N. Variables      2
Criterion      24.20000000      Max Grad Entry  215.6000000

```

Iter	rest	nfun	act	optcrit	difcrit	maxgrad	alpha	slope
1	0	3	0	4.225209	19.97479	12.0012	8e-004	-54227.4
2	0	5	0	4.123006	0.102203	1.46651	1.31975	-0.15465
3	0	9	0	2.952149	1.170858	13.0280	407.726	-3e-003
4	0	11	0	2.748430	0.203719	16.4498	5e-003	-90.5729
5	0	13	0	2.698100	0.050330	16.6332	3e-003	-29.1203
6	0	14	0	2.609541	0.088559	15.7797	4e-003	-33.0735
7	0	15	0	2.504919	0.104622	16.3277	5e-003	-33.9579
8	0	16	0	2.411523	0.093397	17.3825	6e-003	-28.0149
9	0	17	0	2.362683	0.048840	18.8530	8e-003	-19.3104
10	0	19	0	2.347059	0.015624	19.3736	3e-003	-9.20253
11	0	20	0	2.310751	0.036308	19.6798	4e-003	-13.8259
12	0	22	0	2.237142	0.073608	20.2813	8e-003	-17.5790
13	0	24	0	2.202357	0.034785	20.7744	6e-003	-11.4053
14	0	25	0	2.168168	0.034190	21.2433	6e-003	-10.8573

15	0	26	0	2.137800	0.030368	21.7134	7e-003	-10.1502
16	0	27	0	2.113663	0.024137	22.2011	7e-003	-9.29385
17	0	28	0	2.097332	0.016331	22.7153	7e-003	-8.37092
18	0	30	0	2.083319	0.014013	22.9657	4e-003	-7.41977
19	0	31	0	2.055238	0.028082	23.0764	4e-003	-11.6201
20	0	33	0	1.995047	0.060190	23.2723	7e-003	-16.6854

51	0	82	0	1.2e-005	5.8e-005	0.10173	2e-003	-0.05639
52	0	84	0	3.0e-006	9.0e-006	0.01539	6e-004	-0.02994
53	0	86	0	2.8e-006	2.0e-007	3e-003	0.01278	-3e-005
54	0	88	0	2.8e-006	1.3e-008	2e-003	0.30383	-9e-008
55	0	90	0	2.8e-006	2.7e-008	4e-003	4.54979	-1e-008
56	0	92	0	2.3e-006	4.7e-007	0.02129	1.85485	-5e-007
57	0	94	0	5.0e-007	1.8e-006	0.01871	0.02257	-2e-004
58	0	96	0	1.3e-007	3.8e-007	5e-003	1e-003	-5e-004
59	0	98	0	1.1e-007	1.8e-008	8e-004	6e-003	-6e-006

Successful Termination After 59 Iterations
 ABSGCONV convergence criterion satisfied.
 Criterion 1.1014e-007 Max Grad Entry 0.000777436
 Slope SDirect. -5.8224e-006
 N. Function Calls 99 N. Gradient Calls 99
 Preproces. Time 0 Time for Method 0
 Effective Time 0

```
print "UNScaled Fletcher-Reeves Procedure";
mopt = [ "tech" "congra" ,
        "upd"   "fr" ];
< xr, rp> = nlp(frosbr1,x0,mopt,,,,,grosbr);
```

Conjugate-Gradient Optimization
 Fletcher & Reeves Update (Fletcher, 1980, 4.1.4)
 User Specified Gradient

Iteration Start:
 N. Variables 2
 Criterion 24.20000000 Max Grad Entry 215.6000000

Iter	rest	nfun	act	optcrit	difcrit	maxgrad	alpha	slope
1	0	5	0	4.128117	20.07188	1.55692	8e-004	-54227.4
2	0	11	0	2.848166	1.279950	12.1975	0.43624	-3.15335

3	0	14	0	2.648745	0.199422	14.5428	2e-003	-194.176
4	0	19	0	2.515573	0.133171	14.5202	7e-004	-332.107
5	0	24	0	2.422893	0.092681	14.7083	5e-004	-381.612
6	0	29	0	2.350554	0.072339	15.8808	3e-004	-403.521
7	0	36	0	2.283377	0.067177	16.9342	3e-004	-431.541
8	0	43	0	2.232105	0.051272	17.7922	2e-004	-408.278
9	0	50	0	2.187037	0.045067	18.5227	2e-004	-407.317
10	0	57	0	2.146450	0.040587	19.1559	2e-004	-406.614
11	0	64	0	2.109106	0.037344	19.7124	2e-004	-407.605
12	0	71	0	2.074072	0.035033	20.2064	2e-004	-411.182
13	0	78	0	2.040616	0.033457	20.6483	2e-004	-417.956
14	0	83	0	2.008235	0.032381	21.0080	1e-004	-428.395
15	0	88	0	1.972465	0.035770	21.3331	1e-004	-466.679
16	0	93	0	1.936408	0.036057	21.6244	1e-004	-486.531
17	0	98	0	1.899928	0.036480	21.8835	1e-004	-509.252
18	0	103	0	1.862564	0.037364	22.1107	1e-004	-537.438
19	0	108	0	1.823815	0.038749	22.3052	1e-004	-571.786
20	0	113	0	1.783149	0.040666	22.4651	1e-004	-612.851
.....								
70	0	304	0	3.5e-007	1.5e-006	0.01295	3e-003	-1e-003
71	0	307	0	2.0e-007	1.6e-007	3e-003	2e-003	-2e-004
72	0	310	0	1.9e-007	8.4e-009	9e-004	2e-003	-1e-005

Successful Termination After 72 Iterations
 ABSGCONV convergence criterion satisfied.
 Criterion 1.8770e-007 Max Grad Entry 0.000885977
 Slope SDirect. -1.1068e-005
 N. Function Calls 311 N. Gradient Calls 166
 N. Line Searches 72 Preproces. Time 0
 Time for Method 0 Effective Time 0

3 New Developments

3.1 Function codapp

`< x, lind> = codapp(a,b,<,sopt>)`

Purpose: The complete orthogonal decompositon of $m \times n$ matrix \mathbf{A} is:

$$\mathbf{A} = \mathbf{Q} \begin{bmatrix} \mathbf{R}^{-1} \\ \mathbf{0} \end{bmatrix} \mathbf{\Pi}^T \mathbf{V}^T$$

This function computes the $n \times p$ matrix \mathbf{X} :

$$\mathbf{X} = \mathbf{V} \mathbf{\Pi} \begin{bmatrix} \mathbf{R}^{-1T} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{bmatrix} \mathbf{Q}^T \mathbf{B}$$

which is the minimum length solution of a rank-deficient linear least-squares problem:

$$\min_{\mathbf{X}} \|\mathbf{A} - \mathbf{B}\mathbf{X}^T\|_2$$

For full rank \mathbf{A} , the $n \times n$ matrix \mathbf{V} is the identity matrix and the solution \mathbf{X} is unique. The matrix $\mathbf{\Pi}$ is a permutation matrix. For rank deficient matrix \mathbf{A} , $m \geq n$, a solution \mathbf{X} is not unique without additional constraint(s), like that of minimum length.

Input: **a** Numeric (real or complex) $m \times n$ matrix \mathbf{A} .

b Numeric (real or complex) $m \times p$ matrix \mathbf{B} .

sopt is a string option specifying one of two algorithms:

”old” an older algorithm which was already available and should be used together with the LAPACK option.

”new” a newly developed algorithm.

At this time no sufficient test computations were made to determine which of the algorithms is the preferred one.

Output: The following matrices are returned:

prqb Returns the $n \times p$ matrix \mathbf{X} .

lind Gives the integer number of rank deficiencies. For full rank of \mathbf{A} , $rank(\mathbf{A}) = \min(m, n)$, **lind** is zero. Therefore we obtain $rank(\mathbf{A}) = \min(m, n) - lind$.

Restrictions: 1. No missing values or string data are permitted for arguments **a** and **b**.

2. Arguments **a** and **b** must have the same number of rows.

Relationships:

Examples: 1. Simple Example from function cod:

The following 4×4 matrix \mathbf{A} has $\text{rank}(\mathbf{A}) = 2$

```
options nolapack;
b = [ 1 2,
      3 4,
      5 6,
      7 8];
a = b * b';
nr = nrow(a); nc = ncol(a);

< x, lind > = codapp(a,b,"new");
print "X=", x; print "Lind=", lind;
```

```
X=
 |          1          2
-----
 1 |  -1.0000   0.85000
 2 |  -0.50000  0.45000
 3 |  -6e-015   0.05000
 4 |   0.50000  -0.35000
```

Lind= 2

Check this result with the cod function:

```
< qtb, r, v, p, lind > = cod(a,b,"new");
rank = nc - lind;
print "Qtb=", qtb; print "R=", r; print "V=", v;
print "Piv=", p; print "Lind=", lind;
```

```
Qtb=
 |          1          2
-----
 1 |  -9.1530  -10.947
 2 |   0.47186 -0.41287
 3 |   3e-015  -1e-015
 4 |   3e-015  -2e-015
```

```
R=
U |          1          2          3          4
-----
 1 |   181.25   92.760   0.00000   0.00000
```

```

2 |      0  0.44138  0.00000  0.00000
3 |      0      0  0.00000  0.00000
4 |      0      0      0  0.00000

```

```

V=
  |      1      2      3      4
-----
1 | -0.83666  0.23905 -0.11952 -0.47809
2 |  0.00000 -0.80178 -0.53452 -0.26726
3 | -0.19044 -0.50974  0.82903 -0.12886
4 | -0.51355 -0.20042 -0.11271  0.82668

```

```

Piv=
  |  1  2  3  4
-----
1 |  0  1  0  0
2 |  0  0  1  0
3 |  0  0  0  1
4 |  1  0  0  0

```

Lind= 2

```

if (rank < nc) {
  r2 = r[1:rank,1:rank];
  rinv = inv(r2);
  rinv = (rinv -> cons(rank,lind,0.)) |> cons(lind,nc,0.);
  print "Rinv=",rinv;
} else {
  rinv = inv(r);
}
x2 = p * v' * rinv' * qtb;
res = x - x2;
print "Res=", res;
ss1 = ssq(res); print "SS1=",ss1;

```

```

Res=
  |      1      2
-----
1 |  0.000e+000 -1.110e-016
2 | -5.551e-017  0.000e+000
3 | -3.469e-018  1.388e-017
4 |  1.110e-016  5.551e-017

```


SS1= 3.102e-032

3.2 Function hbaddtst

```
gof = hbaddtst(data<,optn>)
```

Purpose: Test for additivity by Tukey (Nollau, 1975, chapter 4.5, A4.2) for the ANOVA model I.2:

$$y_{i,k} = \mu + \alpha_i + \beta_k + E_{i,k}$$

Input: data The $na \times nb$ data matrix is cross frequency table for two nominal scaled variables (factors) with na and nb levels.

optn specifies a vector of options:

1. Controls the printed output. Default is 0, i.e. no printed output.
2. The probability α , default is $\alpha = 0.05$.

Output: There is only one return argument, the vector **gof**. The entries of the vector have the following meaning:

1. Indicating error return of the function. No error means zero.
2. T test value
3. F quantile of $F(\alpha, 1, (na - 1)(nb - 1) - 1)$ distribution
4. p probability for test value T
5. $df1 = 1$
6. $df2 = (na - 1)(nb - 1) - 1$

Restrictions:

1. The input data cannot have missing values.
2. Test is suitable for method 2 of ANOVA model I.

Relationships: `anova()`, `glm()`

Examples:

1. Example by Nollau, p. 211:

```
print "Additivitaetstest by Tukey: p. 211 and 221";
print "Model I.2: Y[i,k]= mu + alfa[i] + beta[k] + E[i,k]";
data = [ 4203 4201 4197 4198 4196 ,
         4205 4206 4201 4201 4200 ,
         4207 4208 4202 4194 4197 ,
         4206 4201 4211 4203 4194 ,
         4212 4204 4201 4202 4198 ,
         4222 4209 4211 4203 4201 ,
         4221 4219 4213 4214 4201 ,
```

```

4214 4216 4202 4193 4198 ,
4226 4217 4214 4215 4201 ,
4217 4218 4206 4214 4213 ];
optn = 2;
gof = hbaddtst(data,optn);
print "GOF=", gof;

```

```

*****
Additivity Test by Tukey
*****

```

```

Model Y[j,k] = Mu + Alpha[j] + Beta[k] + Gamma[j,k] + E[j,k]
F=2.13667 <= F(0.95;1,35)=4.12134:
H: All Gamma[j,k] = 0 cannot be rejected, p=0.152735

```

```

GOF=
-----|-----
          |          1
Error    | 0.00000
Test     | 2.1367
F Quantile | 4.1213
Probability | 0.15273
NDF1     | 1.00000
NDF2     | 35.000
unused   | 0.00000
unused   | 0.00000

```

3.3 Function hbanova

```
< gof,hyp,ci > = hbanova(data<,freq<,optn>>)
```

Purpose: Implements the following nine different methods of analysis of variance for models I and II (Nollau, chapters 4 and 7, A4.3, A4.4):

1. Model I.1: Einfache Klassifikation: (A,B) B: Wiederholungen $Y[i,k]$
 $= \mu + A[i] + E[i,k]$
2. Model I.2: Zweifache Klassifikation ohne Wiederholungen (Kreuzklassifikation): (A,B) B: Levels of categorical variable $Y[i,k] = \mu + A[i] + B[k] + E[i,k]$
3. Model I.3: Zweifache Klassifikation mit Wiederholungen (Kreuzklassifikation): (A,B,C) B: Levels of categorical variable C: equal number Wiederholungen $Y[i,k,l] = \mu + A[i] + B[k] + G[i,k] + E[i,k,l]$

4. Model I.4: Dreifache Klassifikation ohne Wiederholungen: (A,B,C) B: Levels of categorical variable C: Levels of categorical variable $Y[i,k,l] = \mu + A[i] + B[k] + G[l] + C[i,k] + D[i,l] + Z[k,l] + E[i,k,l]$
5. Model II.5: Einfache Klassifikation orthogonal: (A,B) B: Wiederholungen $Y[i,k] = \mu + A[i] + E[i,k]$
6. Model II.6: Einfache Klassifikation nicht orthogonal: (A,B) B: Wiederholungen $Y[i,k] = \mu + A[i] + E[i,k]$
7. Model II.7: Zweifache Klassifikation hierarchisch: (A,B,C) B: Levels of categorical variable C: equal number Wiederholungen $Y[i,k,l] = \mu + A[i] + B[i,k] + E[i,k,l]$
8. Model II.8: Zweifache Klassifikation ohne Wiederholungen (Kreuzklassifikation): (A,B) B: Levels of categorical variable $Y[i,k] = \mu + A[i] + B[k] + E[i,k]$
9. Model II.9: Zweifache Klassifikation mit Wiederholungen (Kreuzklassifikation): (A,B,C) B: Levels of categorical variable C: Wiederholungen $Y[i,k,l] = \mu + A[i] + B[k] + C[i,k] + E[i,k,l]$

For all models the factor A is a categorical variable with `na` levels. The factors B and C can be either the levels of a categorical variable or the replications depending on the analysis model.

Input: data The input data object may be a vector, a $na \times nb$ matrix, or a $na \times nb \times nc$ tensor.

freq This is a frequency vector which should be specified only for models I.1 or II.6.

optn specifies a vector of options:

1. Controls the printed output. Default is 0, i.e. no printed output.
2. The probability α , default is $\alpha = 0.05$.
3. Specifies an integer model number inbetween 1 and 9 to select one of the models mentioned above.

Output: There are no more than three return arguments,

gof a vector with entries having the following meaning:

1. Indicating error return of the function. No error means zero.

hyp Returns a table of the results of hypothesis.

ci Returns confidence intervals for model II parameters.

Restrictions: 1. The input data cannot have missing values.

2. .

Relationships: `anova()`, `glmod()`

Examples: 1. ANOVA Model 1.1: $Y[i,k] = \mu + \text{alfa}[i] + E[i,k]$:

```

data = [ 11.2 11.8  6.3 17.5 14.9  1.6 ,
         8.9  9.2  3.6 14.3 12.9  2.4 ,
         7.3  7.1  3.7 12.6 17.1  3.8 ,
         8.8  7.6  6.0 10.9 17.6  4.2 ,
        11.1 10.7  9.7 12.3 20.2  7.3 ,
        12.3 12.4 11.6 13.6 19.1 11.9 ,
        12.7 14.4 13.2 12.2 20.4 16.8 ,
        13.1 14.6 13.4 14.0 20.4 15.1 ,
        13.2 12.0  9.7 14.3 17.9  9.1 ,
        12.7 10.2  6.7 15.8 17.9  4.4 ,
        14.8 12.2  6.2 18.7 20.1  4.5 ,
        13.1 14.0  7.6 17.2 16.0  2.2 ];

print "ANOVA Model I.1, p.195";
nr = nrow(data); freq = cons(nr,1,6.);
optn = [ 2, .05, 1 ];
< gof,hyp > = hbanova(data,freq,optn);
print "GOF=", gof;
print "Hypothesis=", gof;

```

For models I.1 and I.3 a preliminary Bartlett test is executed:

```

*****
Bartlett Test: Equality of All Variances
*****

Model  $Y[j,k] = \mu + \alpha[j] + E[j,k]$ 

ChiSqu=8.26955 <= ChiSqu(0.95;11)=19.6751:
H: Equal Variances cannot be rejected: p=0.688974

```

```

*****
Variance Analysis Model I.1
*****

```

```

Hypothesis: ALPHA[I] = 0
F=1.36706 <= F(0.95;11,60)=1.95221:
Hypothesis cannot be rejected: p=0.212188

```

2. ANOVA Model 1.2: $Y[i,k] = \mu + \alpha[i] + \beta[k] + E[i,k]$:

```

data = [ 4203 4201 4197 4198 4196 ,
         4205 4206 4201 4201 4200 ,
         4207 4208 4202 4194 4197 ,
         4206 4201 4211 4203 4194 ,
         4212 4204 4201 4202 4198 ,
         4222 4209 4211 4203 4201 ,
         4221 4219 4213 4214 4201 ,
         4214 4216 4202 4193 4198 ,
         4226 4217 4214 4215 4201 ,
         4217 4218 4206 4214 4213 ];

freq = .;
optn = [ 2, .05, 2 ];
< gof,hyp > = hbanova(data,freq,optn);
print "GOF=", gof;
print "Hypothesis=", hyp;

```

For model I.2 a preliminary Tukey test is executed:

```

*****
Additivity Test by Tukey
*****

Model Y[j,k] = Mu + Alpha[j] + Beta[k] + Gamma[j,k] + E[j,k]
F=2.13667 <= F(0.95;1,35)=4.12134:
H: All Gamma[j,k] = 0 cannot be rejected, p=0.152735

```

```

*****
Variance Analysis Model I.2
*****

Hypothesis: ALPHA[I] = 0
F=8.24997 > F(0.95;9,36)=2.15261:
Hypothesis is rejected: p=1.56402e-006

Hypothesis: BETA[J] = 0
F=13.82 > F(0.95;4,36)=2.63353:
Hypothesis is rejected: p=6.34246e-007

```

3. ANOVA Model I.3: Tensor data p. 224:

```

print "Cross Classification with Equal Number Replications";
print "Y[i,k] = mu + alfa[i] + beta[k] + gamma[i,k] + E[i,k]";

```

```

/* Input are Tensor Data d[na,nb,nc]: nc are replications */
real d[5,6,2];
d[1,,]= [ 81.0 80.7, 146.6 100.4, 82.3 103.1,
          119.8 98.9, 98.9 66.4, 86.9 67.7 ];
d[2,,]= [ 105.4 82.3, 142.0 115.5, 77.3 105.1,
          121.4 61.9, 89.0 49.9, 77.1 66.7 ];
d[3,,]= [ 119.7 80.4, 150.7 112.2, 78.4 116.5,
          124.0 96.2, 69.1 96.7, 78.9 67.4 ];
d[4,,]= [ 109.7 87.2, 191.5 147.7, 131.3 139.9,
          140.8 125.5, 89.3 61.9, 101.8 91.8 ];
d[5,,]= [ 98.3 84.2, 145.7 108.1, 89.6 129.6,
          124.8 75.7, 104.1 80.3, 96.0 94.1 ];
freq = .; optn = [ 2 .05 3 ];
< gof,hyp > = hbanova(d,freq,optn);
print "GOF=", gof;
print "Hypothesis=", hyp;

```

```

*****
Bartlett Test: Equality of All Variances
*****

```

Model $Y[j,k] = \mu + \alpha[j] + E[j,k]$

ChiSqu=18.2304 <= ChiSqu(0.95;29)=42.557:
H: Equal Variances cannot be rejected: p=0.939442

```

*****
Variance Analysis Model I.3
*****

```

Hypothesis: ALPHA[I] = 0
F=2.89247 > F(0.95;4,30)=2.68963:
Hypothesis is rejected: p=0.0388184

Hypothesis: BETA[J] = 0
F=9.24762 > F(0.95;5,30)=2.53355:
Hypothesis is rejected: p=2.07543e-005

Hypothesis: ALPHA - BETA[I,J] = 0
F=0.482954 <= F(0.95;20,30)=1.93165:
Hypothesis cannot be rejected: p=0.953458

GOF=

| 1

```

-----
      Error | 0.00000
      Mean | 101.09
     Mean_A | 2.8925
     Mean_B | 9.2476
     Mean_C | .
    Mean_A*B | 0.48295
    Mean_A*C | .
    Mean_B*C | .
     Sigma_A | .
     Sigma_B | .
     Sigma_C | .
     Sigma_E | 458.95
      Rho_1 | .
      Rho_2 | .
Bartl_Test | 18.230
Bartl_Qunt | 42.557
Bartl_Prob | 0.93944
   unused | 0.00000
   unused | 0.00000
   unused | 0.00000

```

Hypothesis=

	Test Value	Ndf1	Ndf2
ALPHA[I] = 0	2.8925	4.0000	30.000
BETA[J] = 0	9.2476	5.0000	30.000
ALPHA - BETA[I,J] = 0	.	.	.
ALPHA - GAMMA[I,K] = 0	0.48295	20.000	30.000
BETA - GAMMA[J,K] = 0	.	.	.

	Fquantile	Probability
ALPHA[I] = 0	2.6896	0.0388
BETA[J] = 0	2.5336	0.0000
ALPHA - BETA[I,J] = 0	.	.
ALPHA - GAMMA[I,K] = 0	1.9317	0.95346
BETA - GAMMA[J,K] = 0	.	.

4. ANOVA Model I.4: p. 374:

```

print "3-Way Classification without replications";
print "Y[i,k,l] = mu + a[i] + b[k] + g[l] + d[i,k] + e[i,l] + z[k,l] + E[i,k,l]";

```

```
print "No Data Example in Book";
```

5. ANOVA Model II.5: p. 284, chapter 7.1:

```
print "1-way Classification: Orthogonal Case";  
print "Equal number replications";  
print "Y[i,k] = mu + A[i] + E[i,k]";  
freq = .; optn = [ 2 .05 5 ];  
print "No Data Example in Book";
```

6. ANOVA Model II.6: p. 284, chapter 7.1:

```
print "1-way Classification: Nonorthogonal Case";  
print "Y[i,k] = mu + alfa[i] + E[i,k]";  
data = [ 727.7 769.0 , 644.8 634.6 ,  
         1138.3 906.7 , 723.2 679.6 ,  
         590.6 646.6 ];  
freq = [ 2 2 2 2 2 ]; optn = [ 2 .05 6 ];  
< gof,hyp,ci > = hbanova(data,freq,optn);  
print "GOF=", gof;  
print "Hypothesis=", hyp;  
print "Confidence Intervals=", ci;
```

```
*****  
Variance Analysis Model II.6  
*****
```

```
Mean = 746.11 (Sigma_A)**2 = 52988.7  
      (Sigma_E)**2 = 6048.52  
Intra Class Correlation: 0.795094
```

```
Hypothesis: (SIGMA_A)**2 = 0  
F=8.76059 > F(0.95;4,5)=5.19217:  
Hypothesis is rejected: p=0.0175639
```

```
optn = [ 2 .01 6 ];  
< gof,hyp,ci > = hbanova(data,freq,optn);  
print "GOF=", gof;  
print "Hypothesis=", hyp;  
print "Confidence Intervals=", ci;
```

```
*****  
Variance Analysis Model II.6
```

Mean = 746.11 (Sigma_A)**2 = 52988.7
(Sigma_E)**2 = 6048.52
Intra Class Correlation: 0.795094

Hypothesis: (SIGMA_A)**2 = 0
F=8.76059 <= F(0.99;4,5)=11.3919:
Hypothesis cannot be rejected: p=0.0175639

7. ANOVA Model II.7: p. 298, 303, chapter 7.3:

```
print "Hierarchical Classification: Equal Number Replications";
print "Y[i,k,l] = mu + A[i] + B[i,k] + E[i,k,l]";
real d[10,2,2];
d[ 1,,] = [ 59.8 61.2, 60.0 65.0 ];
d[ 2,,] = [ 65.0 65.8, 64.5 64.5 ];
d[ 3,,] = [ 65.0 65.2, 65.5 63.5 ];
d[ 4,,] = [ 62.5 61.9, 60.9 61.5 ];
d[ 5,,] = [ 59.8 60.9, 56.0 57.2 ];
d[ 6,,] = [ 68.8 69.0, 62.5 62.0 ];
d[ 7,,] = [ 65.2 65.5, 61.0 59.3 ];
d[ 8,,] = [ 59.6 58.5, 62.3 61.5 ];
d[ 9,,] = [ 61.0 64.0, 73.0 71.7 ];
d[10,,] = [ 65.0 64.0, 62.0 63.0 ];
```

```
freq = .; optn = [ 2 .05 7 ];
< gof,hyp,ci > = hbanova(d,freq,optn);
print "GOF=", gof;
print "Hypothesis=", hyp;
print "Confidence Intervals=", ci;
```

Variance Analysis Model II.7

Mean = 63.115 (Sigma_A)**2 = 2.12014
(Sigma_B)**2 = 9.37175 (Sigma_E)**2 = 1.3205
Intra Class Correlations 0.896936 and 0.165476

Hypothesis: (SIGMA_A)**2 = 0
F=1.42268 <= F(0.95;9,10)=3.02038:
Hypothesis cannot be rejected: p=0.294493

Hypothesis: (SIGMA_B)**2 = 0
 F=15.1942 > F(0.95;10,20)=2.34788:
 Hypothesis is rejected: p=2.90441e-007

Confidence Interval for Mean
 Value=63.115 Lower Bound=61.204 Upper Bound=65.026

Confidence Interval for (Sigma_E)**2
 Value=1.3205 Lower Bound=0.772909 Upper Bound=2.75369

Confidence Interval for (Sigma_B)**2 / (Sigma_E)**2
 Value=7.09712 Lower Bound=2.23901 Upper Bound=25.4711

GOF=

	1
Error	0.00000
Mean	63.115
Mean_A	28.545
Mean_B	20.064
Mean_C	51.250
Mean_A*B	.
Mean_A*C	.
Mean_B*C	.
Sigma_A	2.1201
Sigma_B	9.3717
Sigma_C	.
Sigma_E	1.3205
Rho_1	0.89694
Rho_2	0.16548
unused	0.00000
unused	0.00000

Hypothesis=

	Test Value	Ndf1	Ndf2
(SIGMA_A)**2 = 0	1.4227	9.0000	10.0000
(SIGMA_B)**2 = 0	15.194	10.0000	20.000
(SIGMA_AB)**2 = 0	.	.	.

	Fquantile	Probability
(SIGMA_A)**2 = 0	3.0204	0.29449

```
(SIGMA_B)**2 = 0 |      2.3479      3e-007
(SIGMA_AB)**2 = 0 |      .          .
```

Confidence Intervals=

	Value	Lower CI	Upper CI
CI Mean	63.115	61.204	65.026
CI (Sigma_E)**2	1.3205	0.77291	2.7537
CI (Sigma_B)**2 / (Sigma_E)**2	7.0971	2.2390	25.471

8. ANOVA Model II.8: p. 292, chapter 7.2:

```
print "Cross Classification: Without Replications";
print "Y[i,k] = mu + A[i] + B[k] + E[i,k]";
freq = .; optn = [ 2 .05 8 ];
print "No Data Example in Book";
```

9. ANOVA Model II.9: p. , chapter 7.2:

```
print "Cross Classification: Equal Number Replications";
print "Y[i,k,1] = mu + A[i] + B[k] + C[i,k] + E[i,k,1]";
freq = .; optn = [ 2 .05 9 ];
print "No Data Example in Book";
```

3.4 Function hbbartlett

```
gof = hbbartlett(data<,freq<,optn>>)
```

Purpose: The Bartlett test (Nollau, chapter 4.4, A4.1) can be used in connection with the ANOVA Model I to test the Hypothesis: $\sigma_1^2 = \dots = \sigma_m^2$ for m independent samples from a normal distributed population with size $n_i \geq 2$, $i = 1, \dots, m$. The Bartlett test refers to models I.1 and I.2:

$$Y_{i,k} = \mu + \alpha_i + E_{i,k}$$

Input: data The data set is either an $N = \sum_i^m n_i$ vector or a matrix with m rows and $\max_i n_i$ columns containing the n_i measurements in its first n_i columns.

freq This is a m vector of integer frequencies n_i for the m samples.

optn This argument is optional and should be either a scalar or vector imposing the following run time options:

1. specifies the amount of printed output (default is 0: no printed output)

Output: There is only one return argument, the vector `gof`. The entries of the vector have the following meaning:

1. Indicating error return of the function. No error means zero.
2. T test value
3. χ^2 quantile of $\chi^2(\alpha, m - 1)$ distribution
4. p probability for test value T
5. $df = m - 1$

Restrictions:

1. The input data cannot have missing values.
2. Test is suitable for methods 1 and 3 of ANOVA model I.

Relationships: `anova()`, `hbanova()`, `glmmod()`

Examples: 1. Example by Nollau p. 195:

```
print "Bartlett Test: p. 195: t=8.27, chi=19.7, ndf=11";
print "Model 1.1: Y[i,k]= mu + alfa[i] + E[i,k]";
data = [ 11.2 11.8  6.3 17.5 14.9  1.6 ,
         8.9  9.2  3.6 14.3 12.9  2.4 ,
         7.3  7.1  3.7 12.6 17.1  3.8 ,
         8.8  7.6  6.0 10.9 17.6  4.2 ,
        11.1 10.7  9.7 12.3 20.2  7.3 ,
        12.3 12.4 11.6 13.6 19.1 11.9 ,
        12.7 14.4 13.2 12.2 20.4 16.8 ,
        13.1 14.6 13.4 14.0 20.4 15.1 ,
        13.2 12.0  9.7 14.3 17.9  9.1 ,
        12.7 10.2  6.7 15.8 17.9  4.4 ,
        14.8 12.2  6.2 18.7 20.1  4.5 ,
        13.1 14.0  7.6 17.2 16.0  2.2 ];
nr = nrow(data); freq = cons(nr,1,6.);
optn = 2;
gof = hbbartlett(data,freq,optn);
print "GOF=", gof;
```

```
*****
Bartlett Test: Equality of All Variances
*****
```

Model $Y[j,k] = \text{Mu} + \text{Alpha}[j] + E[j,k]$

ChiSqu=0 <= ChiSqu(0.95;11)=0:

H: Equal Variances cannot be rejected: p=0

```

GOF=
-----|----- 1
      Error | 0.00000
      Test  | 8.2696
ChiSqu Quant | 19.675
Probability | 0.68897
      NDF  | 11.000
      unused | 0.00000
      unused | 0.00000
      unused | 0.00000

```

3.5 Function hbcover

```
gof = hbcover(ydata,wdata<,freq<,optn<>>)
```

Purpose: There are two models for covariance analysis with one covariable implemented (see Nollau, 1975, chapters 5.1 and 5.2, A5):

1. One way (1,1) classification with one covariable and
2. unrepeatd two way (2,1) classification with one covariable.

Chapter 5.3 also describes the (2,2) classification model.

Input: ydata

1. For (1,1) classification this can be
 - either a vector Y of size ns , where $ns = \sum_j f_j, j = 1, \dots, na$
 - or a $na \times nb$ matrix, where $nb = \text{sum} f_j$
2. For (2,1) classification this is a $na \times nb$ cross frequency table Y of two categorical variables with na and nb levels.

wdata This is a second data object W of the same size as the first input argument Y .

freq valid only (1,1) classification: specifies a vector $f[na]$ of the frequencies f_j of measurements for each level of the data in Y and W .

optn specifies a vector of options:

1. Controls the printed output. Default is 0, i.e. no printed output.
2. The probability α , default is $\alpha = 0.05$.

Output: The only return argument is a vector with the following entries:

1. Indicating error return of the function. No error means zero.
2. Test value for $\gamma = 0$.
3. Test criterion for $\gamma = 0$.

4. Quantile for testing equality of the means of factor A.
5. Criterion for testing equality of the means of factor A.
6. Quantile for testing equality of the means of factor B.
7. Criterion for testing equality of the means of factor B.

Restrictions: 1. The input data cannot have missing values.
2.

Relationships: anova(), glmmod()

Examples: 1. Covariance Analysis: Model (1,1): p. 247:

```
print "Covariance Analysis: Model (1,1): p. 247";
Y = [ 766.8 854.0 1080.0 954.6 802.5 862.5 501.6 417.6 595.2 1033.2 ,
      612.0 942.0 365.2 276.0 731.5 487.2 369.2 498.0 464.8 667.4 ];
W = [ 7.1 7.0 7.5 7.4 7.5 7.5 4.4 4.3 6.2 8.2,
      7.2 6.2 4.4 4.0 7.7 5.6 5.2 5.3 5.6 7.1 ];
Bfrq = [ 10 10 ];
optn = 2;
gof = hbcovar(Y,W,Bfrq,optn);
print "GOF=",gof;
```

```
*****
(1,1) Classification: One factor A=2 with one Covariable
*****
```

Number Replications

1 : 10 10

ABS(T=6.51661) > T(0.975,17)=2.10982:

H: Gamma = 0 is rejected: p=0.999997

F=4.98054 > F(0.95;1,17)=4.45132:

H: Equal Means of Factor A is rejected, p=0.0393832

GOF=

	1
Error	0.00000
TestGamma	6.5166
CritGamma	2.1098
Test_A	4.9805
Crit_A	4.4513
unused	.

2. Covariance Analysis: Model (2,1): p. 254:

```
print "Covariance Analysis: Model (2,1): p. 254";
Y = [ 2.8 1.9 0.8 0.5 2.1 0.9 ,
      3.0 5.4 2.8 1.0 0.5 1.1 ,
      4.5 0.9 1.9 0.1 3.2 3.2 ,
      2.3 0.2 3.3 0.6 2.2 2.8 ];
W = [ 50 49 51 50 50 50 ,
      51 53 53 50 48 48 ,
      52 47 51 49 52 52 ,
      48 45 53 48 50 50 ];
optn = 2;
gof = hbcovar(Y,W,..,optn);
print "GOF=",gof;
```

```
*****
(2,1) Classification: Two factors (A=4,B=6) with one Covariable
*****
```

```
ABS(T=12.6166) > T(0.975,14)=2.14479:
H: Gamma = 0 is rejected: p=1
F=6.72921 > F(0.95;3,14)=3.34389:
H: Equal Means of Factor A is rejected, p=0.00485774
F=19.6477 > F(0.95;5,14)=2.95825:
H: Equal Means of Factor B is rejected, p=7.03401e-006
```

```
GOF=
      |      1
-----|-----
Error  | 0.00000
TestGamma | 12.617
CritGamma | 2.1448
Test_A  | 6.7292
Crit_A  | 3.3439
Test_B  | 19.648
Crit_B  | 2.9582
unused | .
```

3.6 Function hbdiscrim

```
< gof,fsep,yhat,zhat > = hbdiscrim(data,idx<,>,optn<,>,zdat<>>)
```

Purpose: The code in appendix A3 refers only to two sample discriminance

analysis (Nollau, 1975, chapter 6.1). However, chapter 6.2 also treats the general case of $K > 2$ samples.

Input: data The input data is in the form of a $nr \times nc$ matrix which contains a identity column. The identity column determines to which sample the observation belongs. The discriminance analysis is then performed w.r.t. only $nc - 1$ columns of the data matrix.

idc specifies the number of the identity column. (The data of this column is not included in the analysis.)

optn specifies a vector of options:

1. Controls the printed output. Default is 0, i.e. no printed output.
2. The probability α , default is $\alpha = 0.05$.
3. If entry three is set unequal zero, then the additional data set **zdat** also contains a column **idc** specifying priors. If this entry is missing or zero, then **zdat** does not contain priors.

zdat specifies an additional data set with either nc or $nc - 1$ columns (see **optn**()).

Output: gof The entries of this vector have the following meaning:

1. Indicating error return of the function. No error means zero.
2. The second entry contains the separation threshold for the posteriors.
3. The third entry gives the Mahalanobis test value.
4. The fourth entry gives the corresponding critical F value.
5. The fifth entry gives the p value.

fsep is a vector of $nv = nc - 1$ coefficients of the linear separator function.

yhat This is a vector of nr values computed as the predicted values of the separator function and which permits the prediction of the sample.

zhat This is a vector of predicted function values for the **zdat** input data matrix.

- Restrictions:**
1. The input data cannot have missing values.
 2. The columns of **data** and **zdat** must be compatible except for the **idc** column.

Relationships: `discrim()`

Examples: 1. Discriminance Analysis: p. 267:

```
X = [ 63.6  2.096 1, 59.2  2.048 1, 59.2  2.144 1, 64.4  2.256 1,
      64.0  2.064 1, 65.6  2.264 1, 66.4  2.144 1, 66.8  1.984 1,
      67.2  2.192 1, 67.6  2.240 1, 67.2  2.032 1,
      60.0  1.952 2, 56.0  1.856 2, 56.4  1.984 2, 57.6  1.920 2,
      59.6  2.032 2, 57.2  2.016 2, 56.4  1.984 2, 54.4  1.984 2,
```



```
50.4 1.776 2, 45.6 1.616 2, 54.8 1.680 2 ];
```

```
optn = 2;  
< gof,tren,yhat > = hbdisc(X,3,optn);  
print "GOF=",gof;  
print "Tren=",tren;  
print "Yhat=",yhat;
```

```
*****  
Discriminance Aanalysis for K=2 Samples  
*****  
Threshold Separating Samples. . . . . 47.8876  
Mahalanobis Distance. . . . . 7.01903  
Test Value for Mahalanobis Distance . . . . . 18.3372  
Critical F(4.71301e-296,2,19) Value . . . . . 3.52189  
Probability . . . . . 3.66801e-005
```

Linear Discriminance Function

```
          VAR_1      VAR_2  
1  0.590377168  6.200649587
```

Prior and Posterior Probability

```
*****
```

N	Name	Prior	Yhat	Post
1	OBS_01	0	50.54454941	0
2	OBS_02	0	47.64925869	1
3	OBS_03	0	48.24452105	0
4	OBS_04	0	52.00895508	0
5	OBS_05	0	50.58227949	0
6	OBS_06	0	52.76701288	0
7	OBS_07	0	52.49523666	0
8	OBS_08	0	51.73928359	0
9	OBS_09	0	53.26516957	0
10	OBS_10	0	53.79895162	0
11	OBS_11	0	52.27306564	0
12	OBS_12	1	47.52629807	1
13	OBS_13	1	44.56952703	1
14	OBS_14	1	45.59936105	1
15	OBS_15	1	45.91097208	1
16	OBS_16	1	47.78619917	1
17	OBS_17	1	46.27008357	1

```

18 OBS_18      1 45.59936105    1
19 OBS_19      1 44.41860671    1
20 OBS_20      1 40.76736293    1
21 OBS_21      1 36.94144859    1
22 OBS_22      1 42.76976010    1

```

```

*****
Evaluation of Training Data Fit
*****

```

Index	Value	StdErr
Absolute Classification Error	1	.
Classification Accuracy	95.45454545	.
Goodman-Kruskal Gamma	1.00000000	0.00000000
Kendall Tau_a	0.00000000	.
Kendall Tau_b	0.912870929	0.081417368
Stuart Tau_c	0.909090909	0.086678417
Somers D C R	0.909090909	0.086678417
Somers D R C	0.916666667	0.079785592

Classification Table

Observed	Predicted	
	Event	NoEvt
Event	10	1
NoEvt	0	11
Missing	0	0

3.7 Function hblreg

```
< gof,parm,yhat,zhat,test> = hblreg(xdat,ydat<,optn<,zdat<,cont>>>)
```

Purpose: This function implements the common multiple linear least squares regression (a simple version of the `reg` function), see Nollau, 1975, chapters 3.1 to 3.3, A2.2.

Input: `xdat` specifies an $m \times n$ data matrix X where the m rows correspond to observations and the n columns to predictor variables. Note, that the function assumes an intercept column (constant ones) in X .

`ydat` specifies an m response vector.

optn specifies a vector of options:

1. Controls the printed output. Default is 0, i.e. no printed output.
2. The probability α , default is $\alpha = 0.05$.

zdat specifies an additional $r \times n$ data set which should be scored with coefficients computed from (x, y) .

cont The fifth input argument specifies an optional contrast vector of size n .

Output: gof The entries of this vector have the following meaning:

1. Indicating error return of the function. No error means zero.
2. Returns the error variance. Note that the **reg** function computes many more indicators for the goodness of fit.

parm returns the $n \times 3$ matrix with the estimates for coefficients of the linear function together with lower and upper confidence limits.

yhat returns the $m \times 3$ matrix of predicted values \hat{y} together with lower and upper confidence limits.

zhat if the fourth input argument z is specified, this $r \times 3$ matrix contains the predicted values together with lower and upper confidence limits.

test if the fifth input argument *cont* is specified, this n vector returns the test vector for the contrast.

Restrictions: 1. The input data cannot have missing values.

2. The size of input arguments 1,2,4, and 5 must be compatible.

Relationships:

Examples: `reg()`

1. Example p. 137:

```
print "Lineare Regression, p. 137";
x = [ 0 20 40 60 80 100 ];
x = cons(6,1,1.) -> x';
y = [ 70.7 88.3 104.9 124.7 148.0 176.0 ];
optn = 2;
< gof,parm,yhat > = hblreg(x,y,optn);
print "GOF=",gof;
print "Parm=",parm;
print "Yhat=",yhat;
```

```
*****
Linear Regression: Error Variance=19.7842
*****
```

Linear Regression Coefficients

Dense Matrix (2 by 3)

	Estimate	Lower CI	Upper CI
1	66.952381	58.014493	75.890269
2	1.0362857	0.8886813	1.1838901

Predicted Values of Response

Dense Matrix (6 by 3)

	Estimate	Lower CI	Upper CI
1	66.952381	58.014493	75.890269
2	87.678095	80.967911	94.388279
3	108.40381	103.15053	113.65709
4	129.12952	123.87625	134.38280
5	149.85524	143.14505	156.56542
6	170.58095	161.64306	179.51884

GOF=

	1
Error	0.00000
EVariance	19.784
unused	.
unused	.
unused	.
unused	.
unused	.
unused	.

2. Example p. 142:

```
X = [ 6.44  6.44 11.26 11.26 12.87 14.48 16.09 16.09 16.09 17.70
      17.70 19.31 19.31 19.31 19.31 20.92 20.92 20.92 20.92 22.53
      22.53 22.53 22.53 24.14 24.14 24.14 25.74 25.74 27.35 27.35
      28.96 28.96 28.96 28.96 30.57 30.57 30.57 32.18 32.18 32.18
      32.18 32.18 35.40 37.01 38.62 38.62 38.62 38.62 40.23 ];
Y = [ .61  3.05  1.22  6.71  4.88  3.05  7.93  5.49 10.37  8.54
```

```

5.18 6.10 4.27 7.32 8.54 10.37 7.93 10.37 14.03 10.98
7.93 18.30 24.40 16.47 7.93 6.10 9.76 12.20 15.25 12.20
17.08 25.62 23.18 12.81 20.74 14.03 10.98 14.64 17.08 19.52
15.86 9.76 20.13 16.47 28.36 21.35 36.60 28.06 25.92 ];
nr = ncol(X);
X = cons(nr,1,1.) -> X';
optn = 2;
< gof,parm,yhat > = hblreg(X,Y,optn);
print "GOF=",gof;
print "Parm=",parm;
print "Yhat=",yhat;

```

```

*****
Linear Regression: Error Variance=21.8641
*****

```

Linear Regression Coefficients

Dense Matrix (2 by 3)

	Estimate	Lower CI	Upper CI
1	-5.3512523	-9.4850517	-1.2174530
2	0.7493058	0.5912091	0.9074024

Predicted Values of Response

Dense Matrix (49 by 3)

	Estimate	Lower CI	Upper CI
1	-0.5257231	-3.7139053	2.6624591
2	-0.5257231	-3.7139053	2.6624591
3	3.0859308	0.5682040	5.6036575
4	3.0859308	0.5682040	5.6036575
5	4.2923131	1.9858293	6.5987969
6	5.4986954	3.3938525	7.6035383
7	6.7050777	4.7892393	8.6209161
8	6.7050777	4.7892393	8.6209161
9	6.7050777	4.7892393	8.6209161
10	7.9114600	6.1678756	9.6550444
11	7.9114600	6.1678756	9.6550444
12	9.1178423	7.5243200	10.711365

13	9.1178423	7.5243200	10.711365
14	9.1178423	7.5243200	10.711365
15	9.1178423	7.5243200	10.711365
16	10.324225	8.8517720	11.796677
17	10.324225	8.8517720	11.796677
18	10.324225	8.8517720	11.796677
19	10.324225	8.8517720	11.796677
20	11.530607	10.142624	12.918590
21	11.530607	10.142624	12.918590
22	11.530607	10.142624	12.918590
23	11.530607	10.142624	12.918590
24	12.736989	11.389973	14.084006
25	12.736989	11.389973	14.084006
26	12.736989	11.389973	14.084006
27	13.935878	12.582557	15.289200
28	13.935878	12.582557	15.289200
29	15.142261	13.735924	16.548598
30	15.142261	13.735924	16.548598
31	16.348643	14.847421	17.849865
32	16.348643	14.847421	17.849865
33	16.348643	14.847421	17.849865
34	16.348643	14.847421	17.849865
35	17.555025	15.924343	19.185708
36	17.555025	15.924343	19.185708
37	17.555025	15.924343	19.185708
38	18.761408	16.974186	20.548630
39	18.761408	16.974186	20.548630
40	18.761408	16.974186	20.548630
41	18.761408	16.974186	20.548630
42	18.761408	16.974186	20.548630
43	21.174172	19.017099	23.331245
44	22.380555	20.019045	24.742065
45	23.586937	21.012044	26.161830
46	23.586937	21.012044	26.161830
47	23.586937	21.012044	26.161830
48	23.586937	21.012044	26.161830
49	24.793319	21.998146	27.588492

3.8 Function hbltst

```
gof = hbltst(xdat,ydat,freq<,optn>)
```

Purpose: This function implements the linearity test by R. A. Fisher (Nollau, 1975, chapter 2.9, A2.1).

Input: `xdat` specifies an $m \times n$ data matrix X where the m rows correspond to observations and the n columns to predictor variables. Note, that the function assumes an intercept column (constant ones) in X .

`ydat` specifies an m response vector Y .

`optn` specifies a vector of options:

1. Controls the printed output. Default is 0, i.e. no printed output.
2. The probability α , default is $\alpha = 0.05$.

Output: There is only one return argument, the vector `gof`. The entries of the vector have the following meaning:

1. Indicating error return of the function. No error means zero.
2. Test value for the Hypothesis
3. Critical value F value for the test
4. Probability

Restrictions: 1. The input data cannot have missing values.
2.

Relationships:

Examples: 1. Example p. 130:

```
print "Linearitaetstest von R. A. Fisher, p. 130-133";
X = [ 1 240 , 5 240 , 1 280 , 5 280 ];
Y = [ 61.35 63.25 65.60 64.70 67.45 70.85 78.60 74.30 ];
freq = [ 2 2 2 2 ];
```

```
nr = nrow(X); id = cons(nr,1,1.);
X1 = id -> X;
optn = 2;
gof = hbltst(X1,Y,freq,optn);
print "GOF=",gof;
```

```
*****
Test for Linearity by R. A. Fisher
*****
```

```
F=2.29794 <= F(0.95;1,4)=7.70865:
Linearity Hypothesis not rejected (p=0.20413)
```

```
GOF=
      |      1
-----
```

Error		0.00000
Test		2.2979
FQuant		7.7086
Prob		0.20413
unused		.
unused		.

3.9 Function `hbqlrg`

`< gof,parm,yhat > = hbqlrg(xdat,ydat,mpow,freq,<,optn >)`

Purpose: Simple (one predictor) polynomial regression (Nollau, 1975, chapter 3.5, A2.3). There are two versions of the algorithm implemented:

1. The third input argument `mpow` specifies the degree of the polynomial, i.e. coefficients $parm_0, \dots, parm_{mpow}$ are returned.
2. The third input argument `mpow` specifies an upper range for the power. Then the algorithm computes stepwise for $m = 1, \dots, mpow$ each polynomial fit and applies Fisher's linearity test. The algorithm terminates for $m \leq mpow$ with the smallest degree for which the hypothesis of linearity is not rejected.

Note, that the function assumes a 2-column matrix X with constant ones in the first column (intercept).

Input: `xdat` specifies an $m \times 2$ matrix containing constant ones in its first column and the predictor variable in its second column.

`ydat` specifies an *msum* vector of response values.

`mpow` specifies the (maximum) degree of the polynomial.

`freq` specifies a m vector of frequencies $f_i \geq 1$, where $\sum_{i=1}^m f_i = msum$. That means, this vector maps the y_i values to the rows of X .

`optn` specifies a vector of options:

1. Controls the printed output. Default is 0, i.e. no printed output.
2. The probability α , default is $\alpha = 0.05$.
3. If the third entry is not missing and unequal to zero, the third argument specifies the degree of the polynomial and the linearity test is not performed.

Output: `gof` The entries of the vector have the following meaning:

1. Indicating error return.
2. Returns the integer *ndeg* specifying the degree of the computed polynomial.

parm returns the $ndeg + 1$ estimated coefficients c_k of the polynomial $f = c_0 + c_1x + \dots + c_{ndeg}x^{ndeg}$.

yhat Returns a *msum* vector of predicted values.

Restrictions: 1. The input data cannot have missing values and the frequencies should not be smaller than one.

2. The input arguments 1,2, and 4 must be compatible.

Relationships: nlreg(), lreg(), nlp()

Examples: 1. QuasiLineare Regression, p. 165:

```
print "ndeg=2: f2=0.192, Fcrit(.95,8,22)=2.55";
print "alf0= 404.0, alf1=-1.386, alf2=.001";
data = [ 100 230 290 310 , 150 195 240 250 ,
         200 150 190 195 , 250 115 140 145 ,
         300 80 100 105 , 350 60 70 75 ,
         400 40 50 50 , 450 35 40 40 ,
         500 25 30 30 , 550 20 20 20 ,
         600 15 15 15 ];
nr = nrow(data); freq = cons(nr,1,3);
x = data[,1];
y = data[,2:4]; y = shape(y,.,1); /* print "Y=", y; */

print "Specify Degree=2";
grd = 2; optn = [ 2 . 1 ];
< gof,parm > = hbqlreg(x,y,grd,freq,optn);
print "GOF=",gof;
print "Parm=",parm;
```

```
*****
Quasi Linear Regression of Degree 2
*****
```

Coefficients of Polynomial

```
*****
```

Dense Matrix (3 by 3)

| Coefficient F Quantile Crit Value

GRAD_0	404.03030	.	.
GRAD_1	-1.3858741	8.3126949	2.3419373
GRAD_2	0.0012448	0.1918109	2.3965033

```

GOF=
      |          1
-----
Error | 0.00000
Grad  | 2.0000
unused| .
unused| .
unused| .
unused| .

Parm=
      | Coefficient  F Quantile  Crit Value
-----
GRAD_0 |      404.03      .          .
GRAD_1 |     -1.3859      8.3127      2.3419
GRAD_2 |       0.001      0.19181     2.3965

```

```

print "Search for Best Degree in 1,...5";
grd = 5; optn = 2;
< gof,param > = hbqlreg(x,y,grd,freq,optn);
print "GOF=",gof;
print "Parm=",parm;

```

```

*****
Polynomial Regression up to Degree 5 : Found 2
*****

```

```

Coefficients of Polynomial
*****

```

```

Dense Matrix (3 by 3)

```

```

      | Coefficient F Quantile Crit Value
-----
GRAD_0 | 404.03030 0.0000000 .
GRAD_1 | -1.3858741 0.0000000 8.3126949
GRAD_2 | 0.0012448 0.0000000 0.1918109

```

3.10 Function hbrcmp

```
< gof,param> = hbrcmp(x1,y1,x2,y2,<optn>)
```

Purpose: Compare the coefficients of two simple linear regressions (Nollau, 1975, chapter 3.3, A2.4). There are the following three tests provided:

Input: x1 $n_1 \times 2$ matrix for sample 1: containing ones in its first column and one predictor column

y1 n_1 response vector for sample 1

x2 $n_2 \times 2$ matrix for sample 2: containing ones in its first column and one predictor column

y2 n_2 response vector for sample 2

optn specifies a vector of options:

1. Controls the printed output. Default is 0, i.e. no printed output.
2. The probability α , default is $\alpha = 0.05$.

Output: gof

1. n_1 size of sample 1
2. n_2 size of sample 2
3. σ_1^2 test variance for sample 1
4. σ_2^2 test variance for sample 2
5. Test value for $\sigma_1^2 = \sigma_2^2$
6. F quantile for $\sigma_1^2 = \sigma_2^2$
7. Test value for slopes $b_1 = b_2$
8. F quantile for slopes $b_1 = b_2$
9. Test value for intercepts $a_1 = a_2$
10. F quantile for intercepts $a_1 = a_2$

Note, that the test for the equality of intercepts is valid only if the slopes are found different.

parm returns a 2×2 matrix containing the two regression coefficients (intercept a and slope b) for each of the two samples

Restrictions:

1. The input data cannot have missing values.
2. Something is not correct with this implementation. I was not able to confirm the results of the text.

Relationships:

Examples: 1. Compare Variances and Slopes, p. 151:

```
data = [ 925  19.06  19.68 ,   950  18.13  19.07 ,
         975  17.19  18.13 ,   1000 16.56  17.50 ,
        1025 15.84  16.57 ,   1050 14.76  15.93 ,
        1075 13.75  15.06 ,   1100 13.03  14.38 ,
        1125 12.19  13.44 ,   1150 11.25  12.81 ,
        1175 10.42  11.88 ,   1200  9.69  11.27 ];
x = data[,1]; y1 = data[,2]; y2 = data[,3];
nr = nrow(data);
```

```

x = cons(nr,1,1.) -> x;
optn = 2;
< gof,parm > = hbrcmp(x,y1,x,y2,optn);
print "GOF=",gof;
print "Parm=",parm;

```

Compare two Regression Slopes

	Sample 1	Sample 2
Nobs	12	12
Intercept	50.77888112	48.49589744
Slope	-0.034311888	-0.031076923
Error Var	0.011813112	0.006631282

Test for Equality of Error Variances:
 $F=1.78142 \leq F(0.95;11,11)=2.81793$:
H: Equal Variances cannot be rejected: $p=0.176235$

Test for Equality of Slopes:
 $F=50.7097 > F(0.95;1,20)=4.35124$:
H: Equal Slopes is rejected: $p=6.70211e-007$

GOF=

	1
Error	0.00000
Test N1	12.000
Test N2	12.000
Test Var1	0.0118
Test Var2	0.0066
Test Var1=Var2	1.7814
Qunt Var1=Var2	2.8179
Test Slo1=Slo2	50.710
Qunt Slo1=Slo2	4.3512
Test Int1=Int2	.
Qunt Int1=Int2	4.3512
unused	.

Parm=

	1	2

```
-----
1 |    50.779  -0.0343
2 |    48.496  -0.0311
```

3.11 Function `hbscheffe`

```
gof = hbscheffe(data,cont<,>freq<,>optn<>>)
```

Purpose: Scheffè (1959) test (Nollau, 1975, chapter 4.3, A4.5).

Input: data

cont specifies the coefficients of a contrast vector

freq

optn specifies a vector of options:

1. Controls the printed output. Default is 0, i.e. no printed output.
2. The probability α , default is $\alpha = 0.05$.

Output: There is only one return argument, the vector `gof`. The entries of the vector have the following meaning:

1. Indicating error return.

Restrictions: 1. The input data cannot have missing values.

- 2.

Relationships: `anova()`, `hbanova()`

Examples: 1. :

3.12 Function `mds`

```
< gof,conf,... > = mds(data,optn<,>xini<,>wini <,>tra<,>ceq<,>ref<,>pspl<,>sew > .. >)
```

```
< gof,conf,wgt,eval,vec > = mds(data,optn<,>xini,... > .. >)
```

```
< gof,conf,grad,res > = mds(data,optn<,>xini,... > .. >) KYST
```

```
< gof,conf,wgt,res,cov > = mds(data,optn<,>xini,... > .. >) MULTISCALE
```

Purpose: This function implements a variety of *metric* and *nonmetric* methods for 2-way and 3-way multidimensional scaling. Similar to cluster analysis, multidimensional scaling analyzes the relations between the rows of a data set (observations, cases) and is therefore different of most statistical methods which analyze the relations between the columns (variables, items) of a data set.

The result is usually a $n \times d$ configuration matrix $\hat{\mathbf{X}}$ of n points in a small $d \ll p$ dimensional space, whose interpoint distances $d(x_i, x_j)$ fit in some way the distances among the larger p dimensional space of the input data. If $d = 2$ or $d = 3$, the plot of the $n \times d$ result configuration may uncover the most important relations among the observations of the data, such as clusters of similar subjects.

If the data is a tensor consisting of m data matrices belonging to different subjects or treatments different models for the model distance matrix \mathbf{D}_i ,

$$X_i = X * W_i \quad , \text{ for } i = 1, \dots, m$$

can be applied among them:

identity \mathbf{W} is the identity \mathbf{I} matrix. This model can be fitted via KYST and MULTISCALE.

diagonal \mathbf{W} is a $d \times d$ positive diagonal matrix: this model is also known as Horan's model and can be fitted via COSPA, SUMSCAL, INDSCAL, and MULTISCALE.

full (symmetric) model: \mathbf{W} is a $d \times d$ symmetric matrix with a positive diagonal. This model can be fitted by MULTISCALE.

The following estimation methods are implemented:

COSPA 3-way COmmon SPace Analysis by Schoenemann (1972)

INDSCAL 3-way (Metric) INDividual Differences Scaling by Carroll & Chang (1970) using the Canonical Decomposition (CANDECOMP) technique is based on Horan's (1969) model

SUMSCAL 3-way (Metric) individual differences scaling by de Leeuw & Pruzansky (1978)

KYST 2-way Kruskal-Young-Shepard-Torgerson metric and nonmetric scaling; see Young (1987)

MULTISCALE 2- and 3-way maximum likelihood method by Ramsay (1977): this method also computes asymptotic standard errors for the unrotated point coordinates from which ellipsoidal confidence intervals of the point estimates can be drawn

SMACOF 2- and 3-way metric and nonmetric method by de Leeuw (1984, 1994, 2007): these are iterative ALS methods suitable for problems with many observations

Input: data This function permits the following forms of data input:

1. $n \times p$ matrices or $K \times n \times p$ 3-way tables (tensors) of *raw* data.
2. symmetric $n \times n$ matrices or $K \times n \times n$ 3-way tables (tensors) of distance (dissimilarity) data.
3. symmetric $n \times n$ matrices or $K \times n \times n$ 3-way tables (tensors) of correlation, covariance, or scalar product (similarity) data.

optn This argument must be specified in form of a two column matrix where the first column defines the option as string value (in quotes) and the second column can be used for a numeric or string specification of the option. See table below for content.

xini an $n \times d$ matrix of initial values for the **X** configuration of points

Option	Second Column	Meaning
"addc"		add constant if distance data do not satisfy triangle inequality
"dimmax"	int	maximum number dimensions d (def=2)
"dimmin"	int	minimum number dimensions d (def=2)
"dimdif"	int	step size dimensions d (def=1)
"data"	string	kind of input data
	"raw"	$n \times p$ raw data
	"diss"	dissimilarities
	"simi"	similarities
	"dist"	distances
	"corr"	correlations
	"cova"	covariances
	"scp"	scalar product data
"gutlin"		apply Guttman-Lingoes transformation
"met"	string	estimation method
	"torg"	classic Torgerson
	"cos"	COSPA
	"sums"	SUMSCAL
	"inds"	INDSCAL
	"kyst"	KYST
	"mult"	MULTISCALE

Option	Second Column	Meaning
"maxit"	int	number of iterations
"ndim"	int	number dimensions d (def=2)
"noplot"		do not plot
"nopr"		do not print
"pdat"		print input data
"pdis"		print distance matrices
"pcoef"		print X and W configurations
"phis"		print iteration history
"print"	int	controls printed output
"pres"		printed observationwise output
"plotf"	char	plotting into text file (with larger line size)
"plotco"	char	configuration plotting (dimensions pairwise)
	"non"	
	"som"	
	"all"	
"plotsc"	char	scatter plotting (data vs. model)
	"non"	
	"som"	
	"all"	
	"joi"	
"plowgt"	char	subject weights plotting (dimensions pairwise)
	"non"	
	"som"	
	"all"	
"seed"	int	seed of random generator (def: time of day)
"sing"	real	singularity criterion (def=1.e-8)
"xtol"	real	termination criterion (def=1.e-5)

Specific options for the INDSCAL, COSPA, and SUMSCAL methods:

This three methods are specifically designed for the 3-way metric MDS of a set of K scalar product matrices. For input raw data the `mds` function will produce distance or scalar product matrices which are suitable. They only fit 3-way scalar product data in a least squares sense and are therefore rather sensitive to outliers of the data. All other input data types, like (squared) Euclidean distances, are transformed internally to scalar product data.

Option	Second Column	Meaning
"dist"	string	form of distance function
	"euc"	use Euclidean distances (def)
	"squ"	use squared Euclidean distances
"norm"		use normed scalar products
"plin"	int	print only selected steps of INDSCAL iteration

Specific options for the more general KYST methods:

KYST uses more general algorithms and is applicable to a wider range of input data. KYST also permits to fit city-block distances and nonlinear or monotone regression between the data and the model distances. KYST can also deal with a reasonable amount of missing data.

Option	Second Column	Meaning
"acsav"	real	for termination test (def=0.66)
"cutof"	real	threshold for removing small distances from fit
"cosav"	real	for termination test (def=0.66)
"coord"	char	type of normalization
	"as-is"	no normalization
	"stand"	normalize at each iteration
	"rotat"	rotate to principal components (def)
"diag"	char	do or don't use diagonal of data matrix
	"absent"	do not use diagonal
	"present"	use diagonal (def)
"dpow"	real	power of distance function (def=2.) should be in [1., 4.]
"ftol"	real	termination test for stress value (def=.01)
"gtol"	real	termination test for 2-norm of gradient (def=0)
"pre-it"	int	number of iterations for start estimates

Option	Second Column	Meaning
"poldeg"	int	polynomial degree of regression should be in [1, 4]
"regres"	char	type of regression between data and model values
	"asc"	isotone ascending (def)
	"des"	isotone descending
	"poly"	polynomial with intercept
	"poln"	polynomial without intercept
"split"	char	split data values in groups (for unfolding)
	"byrow"	
	"bygroup"	
	"bydeck"	
"sfrm"	int	kind of stress formula for optimization =1: default, =2: for unfolding
"sratst"	real	for termination test (def=.999)
"start"	char	method for initial estimates
	"rand"	random
	"tors"	Torgerson-Young quasi nonmetric
"ties"	char	type of tie processing in isotone regression
	"prim"	type 1 processing
	"seco"	type 2 processing
"unsym"		input of unsymmetric data matrix (does not refer to "data" "raw" input)

Specific options for the MULTISCALE method:

Option	Second Column	Meaning
"alpha"	real	for CI of ML estimation (def=0.05)
"ase"		does compute standard errors (default for MULTISCAL)
"ccorr"		compute and print correlations of log dissimilarities between matrices
"coord"	char	type of normalization
	"as-is"	no normalization
	"rotat"	rotate to principal components (def)
"dlogn"		error distribution: lognormal
"dnorm0"		error distribution: normal with beta=0
"dnorm5"		error distribution: normal with beta=.5
"dnorm1"		error distribution: normal with beta=1
"itxmax"	int	maximum iterations for X (coordinates) optimization
"itwmax"	int	maximum iterations for W (weights) optimization
"itpmax"	int	maximum iterations for P (spline) optimization
"itamax"	int	maximum iterations for A (stand.error) optimization
"knots"	int	number (inner) knots for spline transform (is internally increased by two more boundary knots)
"mod"	char	subjective weighting model
	"ide"	identity model
	"dia"	(positive) diagonal weights
	"ful"	full $d \times d$ weight matrices
"noase"		does not compute standard errors
"orig"	int	=2: use original version of MULTISCALE program =0: use modified version
"pcorr"		print $d \times d$ asymptotic correlation matrices of coordinate estimates
"plis"		print line search information
"ptab"		print some table output
"regres"	char	type of regression between data and model values
	"scale"	
	"power"	power transform
	"spline"	spline transform

Option	Second Column	Meaning
"tech"	char	optimization technique (see NLP)
"vers"	int	version of algorithm
"varobs"	char	stimulus variance level: A fit
	"con"	constant (default)
	"obs"	stimuliwise (fit n add. parameters)
"varsub"	"pair"	pairwise (set $n * (n + 1)/2$ estimates)
	char	subject variance level
	"con"	constant
	"subw"	subjectwise (default) set m add. estimates

The number of parameters $p = p_1 + p_2 + p_3$ for the MULTISCALE approach is:

1. model specification:

$$p_1 = \begin{cases} n * d - d * (d + 1)/2 & \text{identity} \\ n * d + (m - 1) * (d - 1) - d & \text{diagonal} \\ n * d + (m - 1) * d(d + 1)/2 - m - d + 1 & \text{full} \end{cases}$$

2. varobs specification:

$$p_2 = \begin{cases} 0 & \text{constant} \\ n - 1 & \text{stimuliwise} \\ n * n - 1)/2 - 1 & \text{pairwise} \end{cases}$$

3. varsub specification:

$$p_3 = \begin{cases} 0 & \text{constant} \\ m - 1 & \text{subjectwise} \end{cases}$$

Specific options for the SMACOF method:

Option	Second Column	Meaning
--------	---------------	---------

Output: Let $s = \sum_{d=\dimmin}^{\dimmax} d$, i.e. for only one dimensionality $\dimmin = \dimmax$ there is $s = d$.

GOF a vector with some scalar results

conf this is a $n \times s$ matrix containing all of the computed $n \times d$ configurations horizontally concatenated

wgt the $w \times s$ matrix of the individual weights

eval or [i] for INDSCAL, COSPA, SUMSCAL: this a s vector of eigenvalues depending on the method [ii] for KYST, MULTISCAL, and SMACOF:

vec or grad [i] for INDSCAL, COSPA, SUMSCAL: this is a $n \times s$ matrix of eigenvectors [ii] for KYST, MULTISCAL, and SMACOF: it contains the gradient at the solution

Restrictions: 1.

2.

Relationships: cluster(), dist()

Examples: 1. Randomly generated raw data in tensor form $X[2,n,p]$:

```

srand(123);
nind = [ 2 10 10 ]; m = p = nind[1];
nway = size(nind); n = nind[2]; nd = 4;
none = cons(n,1,1.); pone = cons(p,1,1.);

/* [1] Uniform random generation of pxnd weight matrix: W[p,nd] */
wght = rand(p,nd,"g");
print "Uniform: Unscaled wght=",wght;

/* [2] Normal random generated nxnd configuration: X[n,nd] */
coef = rand(n,nd,"g","norm",0.,1.);
coef += rand(n,nd,"g","norm",1.,1.);
mu = cons(nd,1,1.); id = ide(nd);
for (j = 1; j <= n; j++) {
    coef[j,] += mrand("mnor",mu,id)';
}
print "Normal: Unscaled coef=",coef;

```

```

/* [3] Normalize data[p+n,nd]: NORCONF() */
/* [3.1] center X[n,nd] */
mu = coef[+,] / n;

coef = coef - none * mu;
print "Centered Coef=", coef;

/* [3.2] scaling coef[n,nd] */
tv = coef[**,]; rv = 1. ./ sqrt(tv);
coef = coef .* (none * rv);
print "Scaled Coef=", coef;
print "Mean=", coef[+,];
print "Scale=", coef[**,];

/* [3.3] scaling wght[p,nd] */
twgt = wght .* (pone * tv);
print "Scaled WGT=", twgt;

/* [4] Concatenate COEF and WGHT */
wcof = twgt |> coef;

/* [5] Permute dimensions according weights
      sum of squares in descending order */
wscl = twgt[**,];
wrnk = wscl[>:]; print "Ranks=", wrnk;
wcof = wcof[,wrnk];
n1 = p+1; n2 = p+n;
wght = wcof[1:p,]; coef = wcof[n1:n2,];

/* [6] Weighted Configuration: Y = X * W */
real wxdat[p,n,nd];
for (j = 1; j <= p; j++) {
    wv = wght[j,];
    wxdat[j,,] = coef .* (none * wv);
    /* print "WXdat[j,,]=", wxdat[j,,]; */
}
print "Tensor WXDAT=",wxdat;

```

Tensor WXDAT=

```

*****
Tensor wxdat with 3 Dimensions
*****

```

wxdat_1

Dense Matrix (10 by 4)

	1	2	3	4
1	-14.554672	-1.6301023	4.9856908	0.0606599
2	-3.0380098	-4.5080465	1.0150659	0.0439437
3	6.4290345	-7.0272730	0.4288613	-0.6636031
4	-8.4827305	6.9577941	-1.4993646	0.1756061
5	18.784123	1.9255437	3.3502585	0.0904182
6	13.203212	0.4243445	-3.0888729	-0.5465808
7	1.3760075	3.8225599	1.3278726	0.2144417
8	-6.3482351	1.5903091	2.2758083	0.0053984
9	-4.2046344	-5.6754399	-5.2610451	0.3112615
10	-3.1640951	4.1203103	-3.5342749	0.3084545

wxdat_2

Dense Matrix (10 by 4)

	1	2	3	4
1	-6.3948545	-0.7757735	3.4352285	0.2674217
2	-1.3348037	-2.1454008	0.6993982	0.1937275
3	2.8247109	-3.3443127	0.2954930	-2.9255223
4	-3.7270388	3.3112474	-1.0330885	0.7741671
5	8.2531390	0.9163754	2.3083869	0.3986123
6	5.8010665	0.2019476	-2.1282877	-2.4096247
7	0.6045734	1.8191745	0.9149276	0.9453753
8	-2.7892102	0.7568357	1.5680719	0.0237990
9	-1.8473810	-2.7009689	-3.6249525	1.3722094
10	-1.3902016	1.9608753	-2.4351774	1.3598348

(a) Analysis with COSPA:

```
optn = [ "data"      "raw" ,
         "meth"     "cospa" ,
         "ndim"      2 ,
         "norm"      ];
< gof,conf,wgt,eval,vec > = mds(wxdat,optn);
print "GOF=",gof;
print "X Configuration=",conf;
```

```

print "W Configuration=",wgt;
print "Eigenvalues=",eval;
print "Eigenvectors=",evec;

```

```

*****
3-Way Multidimension Scaling
*****

```

```

Raw Input Data
Number Rows of Matrix . . . . . 10
Dimension . . . . . 2
Amount Input Information. . . . . 90
Number of Parameters. . . . . 24
Degrees of Freedom. . . . . 66

```

```

*****
Compute SCHOENEMANN COSPA
*****

```

Eigenvalues of Mean Scalar Product Matrix

```

1 :      0.9573      0.2185      0.1664      0.02963  1.191e-016
6 :  1.633e-017 -1.537e-017 -4.755e-017 -1.052e-016 -3.128e-016

```

Unrotated common space configuration

```

          DIM_1      DIM_2
0_01 -0.465592568  0.071152585
0_02 -0.093331284  0.147963476
0_03  0.227242154  0.246678538
0_04 -0.278491720 -0.215828327
0_05  0.585362887 -0.105058979
0_06  0.434267720 -0.008289568
0_07  0.032286775 -0.137844258
0_08 -0.205208492 -0.042378202
0_09 -0.128315170  0.181828134
0_10 -0.108220302 -0.138223400

```

```

Undiagonalized Weight Matrices:
*****

```

```

Weight matrix:      1

```

```

          DIM_1      DIM_2

```

DIM_1 1.017745116
DIM_2 -0.027635222 0.907661656

Weight matrix: 2

	DIM_1	DIM_2
DIM_1	0.982254884	
DIM_2	0.027635222	1.092338344

Orthogonal Rotation Matrix

	DIM_1	DIM_2
DIM_1	0.230560993	0.973057875
DIM_2	0.973057875	-0.230560993

Rotated common space configuration

	DIM_1	DIM_2
0_01	-0.038111902	-0.469453525
0_02	0.122458472	-0.124931347
0_03	0.292425671	0.164245319
0_04	-0.274222781	-0.221226968
0_05	0.032733382	0.593814469
0_06	0.092058967	0.424478876
0_07	-0.126686370	0.063198410
0_08	-0.088549516	-0.189908979
0_09	0.147344825	-0.166780562
0_10	-0.159450748	-0.073435693

Diagonalized Weight Matrices:

Weight matrix: 1

	DIM_1	DIM_2
DIM_1	0.901113634	
DIM_2	-3.8580e-015	1.024293137

Weight matrix: 2

	DIM_1	DIM_2
DIM_1	1.098886366	
DIM_2	2.1927e-015	0.975706863

Schoenemann's Testindizes for COSPA

Matrix	CommonSpace	Diagonality
1	0.964379639	2.8395e-015
2	0.885697342	1.4974e-015

Result Normalized Configuration

Common Space Configuration

	DIM_1	DIM_2
0_01	-0.489977791	-0.075071833
0_02	-0.130393281	0.241215514
0_03	0.171426039	0.576012484
0_04	-0.230898897	-0.540156903
0_05	0.619775732	0.064477364
0_06	0.443036873	0.181335360
0_07	0.065961412	-0.249543518
0_08	-0.198211702	-0.174422535
0_09	-0.174072122	0.290236005
0_10	-0.076646263	-0.314081938

Subjective Weight Matrices

	DIM_1	DIM_2
W_1	0.940278879	0.232245207
W_2	0.895677733	0.283217434

Goodness-of-fit resp. SCP Matrices

N	Av_SSQ_Diff	Correlation
1	0.000125092	0.994679763
2	0.000660168	0.972705057

Goodness-of-fit resp. Distance Matrices

N	Av_SSQ_Diff	Correlation
1	2.033206077	0.990027529
2	1.716943364	0.965981685

GOF=

| 1

```

-----
Error | 0.00000
Time | 0.00000
Ind. Inf. | 90.000
NParms | 24.000
DF | 66.000
unused | .
unused | .
unused | .
unused | .
unused | .

```

```

X Configuration=
      |      DIM_1      DIM_2
-----
0_01 | -0.48998 -0.07507
0_02 | -0.13039  0.24122
0_03 |  0.17143  0.57601
0_04 | -0.23090 -0.54016
0_05 |  0.61978  0.06448
0_06 |  0.44304  0.18134
0_07 |  0.06596 -0.24954
0_08 | -0.19821 -0.17442
0_09 | -0.17407  0.29024
0_10 | -0.07665 -0.31408

```

```

W Configuration=
      |      DIM_1      DIM_2
-----
W_1 |  0.94028  0.23225
W_2 |  0.89568  0.28322

```

```

Eigenvalues=
      |      DIM_1      DIM_2
-----
1 |  0.95725  0.21846

```

```

Eigenvectors=
      |      DIM_1      DIM_2
-----
0_01 | -0.47588  0.15223
0_02 | -0.09539  0.31657
0_03 |  0.23226  0.52777
0_04 | -0.28464 -0.46177
0_05 |  0.59829 -0.22478

```

```

0_06 | 0.44386 -0.01774
0_07 | 0.03300 -0.29492
0_08 | -0.20974 -0.09067
0_09 | -0.13115 0.38902
0_10 | -0.11061 -0.29573

```

(b) Analysis with SUMSCAL:

We run the same analysis with the SUMSCAL method, but now for two and also one dimension:

```

optn = [ "data"      "raw" ,
        "meth"      "sumsc" ,
        "dimmax"     2 ,
        "dimmin"     1 ,
        "norm"       ];
< gof,conf,wgt,eval,vec > = mds(wxdat,optn);

```

```

*****
3-Way Multidimension Scaling
*****

```

```

                          Raw Input Data
Number Rows of Matrix . . . . . 10
Dimension . . . . . 2
Amount Input Information. . . . . 90
Number of Parameters. . . . . 24
Degrees of Freedom. . . . . 66

```

```

*****
Compute DeLEEUW-PRUZANSKY SUMSCAL
*****

```

Eigenvalues of Mean Scalar Product Matrix

```

-----
1 : 0.9573 0.2185 0.1664 0.02963 1.191e-016
6 : 1.633e-017 -1.537e-017 -4.755e-017 -1.052e-016 -3.128e-016

```

Unrotated common space configuration

```

                          D_2_1      D_2_2
0_01 -0.465592568 0.071152585
0_02 -0.093331284 0.147963476
0_03 0.227242154 0.246678538
0_04 -0.278491720 -0.215828327
0_05 0.585362887 -0.105058979

```

```

0_06  0.434267720 -0.008289568
0_07  0.032286775 -0.137844258
0_08  -0.205208492 -0.042378202
0_09  -0.128315170  0.181828134
0_10  -0.108220302 -0.138223400

```

Undiagonalized Weight Matrices:

Weight matrix: 1

```

          D_2_1      D_2_2
D_2_1  1.017745116
D_2_2 -0.027635222  0.907661656

```

Weight matrix: 2

```

          D_2_1      D_2_2
D_2_1  0.982254884
D_2_2  0.027635222  1.092338344

```

Iterative Simultaneous Diagonalization:

```

Iter  ssq-off-dia    max(ang)    min(cos)
  1   0.055270443   1.3408e+154  0.000000000
  2   4.3715e-016   0.232654169  0.973057875
  3   4.3715e-016   2.8166e-017  1.000000000

```

Residuals SIMDIAG: nit = 2

1 : 4.627e-032 4.93e-032

Orthogonal Rotation Matrix

```

          D_2_1      D_2_2
D_2_1  0.973057875 -0.230560993
D_2_2  0.230560993  0.973057875

```

Rotated common space configuration

```

          D_2_1      D_2_2

```

```

0_01 -0.469453525 -0.038111902
0_02 -0.124931347  0.122458472
0_03  0.164245319  0.292425671
0_04 -0.221226968 -0.274222781
0_05  0.593814469  0.032733382
0_06  0.424478876  0.092058967
0_07  0.063198410 -0.126686370
0_08 -0.189908979 -0.088549516
0_09 -0.166780562  0.147344825
0_10 -0.073435693 -0.159450748

```

Diagonalized Weight Matrices:

Weight matrix: 1

```

          D_2_1      D_2_2
D_2_1  1.024293137
D_2_2 -2.1511e-016  0.901113634

```

Weight matrix: 2

```

          D_2_1      D_2_2
D_2_1  0.975706863
D_2_2 -2.2204e-016  1.098886366

```

Schoenemann's Testindizes for SUMSCAL

```

1  0.964379639  1.5832e-016
2  0.885697342  1.5163e-016

```

Result Normalized Configuration

Common Space Configuration

```

          D_2_1      D_2_2
0_01 -0.489977791 -0.075071833
0_02 -0.130393281  0.241215514
0_03  0.171426039  0.576012484
0_04 -0.230898897 -0.540156903
0_05  0.619775732  0.064477364
0_06  0.443036873  0.181335360
0_07  0.065961412 -0.249543518

```

```

0_08 -0.198211702 -0.174422535
0_09 -0.174072122  0.290236005
0_10 -0.076646263 -0.314081938

```

Subjective Weight Matrices

```

           D_2_1      D_2_2
W_1  0.940278879  0.232245207
W_2  0.895677733  0.283217434

```

Goodness-of-fit resp. SCP Matrices

```

N  Av_SSQ_Diff  Correlation
1  0.000125092  0.994679763
2  0.000660168  0.972705057

```

Goodness-of-fit resp. Distance Matrices

```

N  Av_SSQ_Diff  Correlation
1  2.033206077  0.990027529
2  1.716943364  0.965981685

```

It follows the analysis in one dimension:

```

*****
Compute DeLeeuw-Pruzansky SUMSCAL for 1 Dimension(s)
*****

```

Unrotated common space configuration

```

           D_1_1
0_01 -0.465592568
0_02 -0.093331284
0_03  0.227242154
0_04 -0.278491720
0_05  0.585362887
0_06  0.434267720
0_07  0.032286775
0_08 -0.205208492
0_09 -0.128315170
0_10 -0.108220302

```

Undiagonalized Weight Matrices:

Weight matrix: 1

D_1_1
D_1_1 1.017745116

Weight matrix: 2

D_1_1
D_1_1 0.982254884

Schoenemann's Testindizes for SUMSCAL

1 0.908403857 0.000000000
2 0.816123639 0.000000000

Result Normalized Configuration

Common Space Configuration

D_1_1
O_01 -0.475875172
O_02 -0.095392504
O_03 0.232260793
O_04 -0.284642206
O_05 0.598290617
O_06 0.443858516
O_07 0.032999828
O_08 -0.209740518
O_09 -0.131149009
O_10 -0.110610345

Subjective Weight Matrices

D_1_1
W_1 0.974237878
W_2 0.940264806

Goodness-of-fit resp. SCP Matrices

N Av_SSQ_Diff Correlation

```

1 0.000574718 0.975346430
2 0.001385490 0.941856456

```

Goodness-of-fit resp. Distance Matrices

```

N Av_SSQ_Diff Correlation
1 0.000000000 1.000000000
2 0.000000000 1.000000000

```

(c) Analysis with INDSCAL:

```

optn = [ "data"      "raw" ,
         "meth"     "indsc" ,
         "ndim"      2 ,
         "norm"      ];
< gof,conf,wgt,eval,eval,eval > = mds(wxdat,optn);

```

The following output of the iteration history could be restricted to larger steps using the plin option (default is 10):

Iterative Canonical Decomposition:

Iter	Way	Max. Dev.	Maximum	Residual
1	1	0.092338344		
1	2	0.002573734	0.092338344	0.275733651
11	1	0.000126273		
11	2	0.001420932	0.001420932	0.275619458
21	1	9.1720e-005		
21	2	0.001341886	0.001341886	0.275430703
31	1	5.9351e-005		
31	2	0.001262113	0.001262113	0.275255123
41	1	3.3093e-005		
41	2	0.001178954	0.001178954	0.275097042
.....				
631	1	3.3370e-006		
631	2	1.2614e-005	1.2614e-005	0.274047651
641	1	3.1349e-006		
641	2	1.1837e-005	1.1837e-005	0.274047522
651	1	2.9452e-006		
651	2	1.1108e-005	1.1108e-005	0.274047402
661	1	2.7671e-006		
661	2	1.0426e-005	1.0426e-005	0.274047292
664	0	9.9616e-006	9.9616e-006	0.274047235

Residuals CADECO: nit = 664

1 : 0.006999 0.03625

Result non-normalized configuration X:

Common Space Configuration

	DIM_1	DIM_2
0_01	-0.469705827	-0.036553819
0_02	-0.124329431	0.121437948
0_03	0.164347235	0.294394706
0_04	-0.222344182	-0.271971552
0_05	0.594691055	0.028653940
0_06	0.423981427	0.094048475
0_07	0.063142821	-0.127689246
0_08	-0.190385558	-0.087104099
0_09	-0.165710781	0.144643058
0_10	-0.073686760	-0.159859411

Common Space Configuration

	DIM_1	DIM_2
0_01	-0.469705827	-0.036553819
0_02	-0.124329431	0.121437948
0_03	0.164347235	0.294394706
0_04	-0.222344182	-0.271971552
0_05	0.594691055	0.028653940
0_06	0.423981427	0.094048475
0_07	0.063142821	-0.127689246
0_08	-0.190385558	-0.087104099
0_09	-0.165710781	0.144643058
0_10	-0.073686760	-0.159859411

Subjective Weight Matrices

	DIM_1	DIM_2
W_1	1.023979211	0.899153581
W_2	0.975339995	1.102091165

Result Normalized Configuration

Common Space Configuration

	DIM_1	DIM_2
0_01	-0.489950010	-0.072139585
0_02	-0.129687993	0.239659861
0_03	0.171430553	0.580992970
0_04	-0.231927151	-0.536740493
0_05	0.620322065	0.056549038
0_06	0.442254902	0.185606268
0_07	0.065864258	-0.251996903
0_08	-0.198591120	-0.171901425
0_09	-0.172852867	0.285455541
0_10	-0.076862638	-0.315485272

Common Space Configuration

	DIM_1	DIM_2
0_01	-0.489950010	-0.072139585
0_02	-0.129687993	0.239659861
0_03	0.171430553	0.580992970
0_04	-0.231927151	-0.536740493
0_05	0.620322065	0.056549038
0_06	0.442254902	0.185606268
0_07	0.065864258	-0.251996903
0_08	-0.198591120	-0.171901425
0_09	-0.172852867	0.285455541
0_10	-0.076862638	-0.315485272

Subjective Weight Matrices

	DIM_1	DIM_2
W_1	0.941108062	0.230861820
W_2	0.896405242	0.282966978

Goodness-of-fit resp. SCP Matrices

N	Av_SSQ_Diff	Correlation
1	0.000127246	0.994584218
2	0.000659062	0.972744353

Goodness-of-fit resp. Distance Matrices

N	Av_SSQ_Diff	Correlation
1	2.075138105	0.989819063

2 1.718323923 0.965938432

2. Scalar product and distance data in tensor form $D[2,n,n]$:

The first part of randomly generating the `coef` and `wgt` data is the same as for the raw data tensor `wxdat` above.

The tensor data `eudis` of distances are then obtained using the `dist` function:

```
/* [6] Weighted Euclidean Distances: WEUCDIS() */
real eudis[p,n,n];
for (j = 1; j <= p; j++) {
  wv = wght[j,];
  xcof = coef .* (none * wv);
  optn = [ 0, 0 ];
  eudis[j,,] = dist(xcof,"L2",optn);
  /* print "Eudis[j,,]=", eudis[j,,]; */
}
print "Tensor EUDIS=",eudis;
```

Tensor EUDIS=

```
*****
Tensor eudis with 3 Dimensions
*****
```

```
eudis_1
*****
```

Dense Symmetric Matrix (10 by 10)

S	1	2	3	4	5
1	0.0000000				
2	12.517277	0.0000000			
3	22.152531	9.8394964	0.0000000		
4	12.356763	12.940254	20.551525	0.0000000	
5	33.567743	22.870327	15.553271	28.148374	0.0000000
6	28.987725	17.472745	10.667907	22.715945	8.6757329
7	17.231406	9.4344830	12.034581	10.724700	17.628005
8	9.2229700	7.0525519	15.536413	6.9026711	25.157692
9	15.117752	6.4949865	12.174883	13.858909	25.699440
10	15.344827	9.7586323	15.262637	6.3637807	23.108129

S	6	7	8	9	10
---	---	---	---	---	----

```
-----
6 | 0.0000000
7 | 13.096467 0.0000000
8 | 20.315094 8.0987128 0.0000000
9 | 18.592868 12.836619 10.690362 0.0000000
10 | 16.807093 6.6596174 7.0984902 10.001059 0.0000000
```

```
eudis_2
*****
```

Dense Symmetric Matrix (10 by 10)

```
S |          1          2          3          4          5
-----
1 | 0.0000000
2 | 5.9135599 0.0000000
3 | 10.566485 5.3508700 0.0000000
4 | 6.6365373 6.2318712 10.132854 0.0000000
5 | 14.788985 10.194800 7.9197796 12.671486 0.0000000
6 | 13.704587 8.4382427 5.2512397 10.573009 5.8389505
7 | 7.9080518 4.4822392 6.8526023 4.9812874 7.8457810
8 | 4.3468595 3.3647800 7.6585561 3.8384410 11.074632
9 | 8.6863458 4.5453515 7.4888400 6.8377826 12.298703
10 | 8.2577739 5.2962197 8.4694364 3.0972848 10.840219

S |          6          7          8          9         10
-----
6 | 0.0000000
7 | 7.0806884 0.0000000
8 | 9.6791208 3.7312506 0.0000000
9 | 9.1360795 6.8728797 6.4520669 0.0000000
10 | 8.3133128 3.9235426 4.6062928 4.8329621 0.0000000
```

All the results obtained with COSPA, SUMSCAL, and INDSCAL are the same as those obtained with the raw data input. Here we only show the mds call for COSPA:

```
optn = [ "data"      "dis" ,
         "meth"     "cospa" ,
         "nobs"     10 ,
         "ndim"     2 ,
         "norm"     ];
< gof,conf,wgt,eval,eval,eval > = mds(eudis,optn);
print "GOF=",gof;
```

```

print "X Configuration=",conf;
print "W Configuration=",wgt;
print "Eigenvalues=",eval;
print "Eigenvectors=",evec;

```

The tensor data scalp of scalar products are then obtained using the simple code:

```

/* [6] Weighted Configuration: Y = X * W */
real scalp[p,n,n];
for (j = 1; j <= p; j++) {
  wv = wght[j,];
  xdat = coef .* (none * wv);
  /* print "Xdat=", xdat; */
  scalp[j,,] = xdat * xdat';
}
print "Tensor SCALP=",scalp;

```

Tensor SCALP=

```

*****
Tensor scalp with 3 Dimensions
*****

```

```

scalp_1
*****

```

Dense Symmetric Matrix (10 by 10)

S	1	2	3	4	5
1	239.35651				
2	56.629284	30.584276			
3	-80.019400	12.553964	91.339342		
4	104.65673	-7.1096775	-104.18964	122.64655	
5	-259.82674	-62.342084	108.60925	-150.95050	367.78340
6	-208.29347	-45.183882	80.939938	-104.51143	238.42991
7	-19.625132	-20.055300	-17.588603	12.970976	37.675707
8	101.15092	14.427146	-51.016135	61.504092	-108.55878
9	44.237560	33.032238	10.388312	4.1211227	-107.50639
10	21.733749	-12.535965	-51.017027	60.861770	-63.313758

S	6	7	8	9	10

```

6 | 184.34477
7 | 15.570962 18.314592
8 | -90.174890 0.3669736 48.008505
9 | -41.842453 -34.399568 5.6948546 77.665048
10 | -29.279458 6.7693928 18.597319 8.6092796 39.574698

```

```

scalp_2
*****

```

Dense Symmetric Matrix (10 by 10)

```

S |          1          2          3          4          5
-----
1 | 53.368298
2 | 12.654620 6.9111339
3 | -15.236448 3.0443698 27.809416
4 | 17.923227 -2.7016504 -24.171767 26.521784
5 | -45.452089 -11.290610 19.764048 -29.801599 74.441589
6 | -45.209182 -10.131875 22.131477 -20.618844 42.188651
7 | -1.8816273 -3.8868014 -6.8715051 3.5571455 9.1455204
8 | 22.642510 3.2006496 -10.016078 11.300032 -18.696990
9 | 1.8234916 5.9911013 -1.2710098 2.7489006 -25.542608
10 | -0.6327998 -3.7909387 -15.182503 15.242772 -14.755914

S |          6          7          8          9          10
-----
6 | 44.029056
7 | -0.3506802 5.4057317
8 | -19.422208 1.1477050 10.811910
9 | -6.8538026 -8.0497273 -2.5429844 25.731289
10 | -5.7625912 1.7842387 1.5754542 7.9653492 13.556932

```

Running the following call of mds will generate the same results as reported above for other data input:

```

optn = [ "data"      "scp" ,
         "meth"     "cospa" ,
         "nobs"      10 ,
         "ndim"      2 ,
         "norm"      ] ;
< gof,conf,wgt,eval,vec > = mds(scalp,optn);

```

3. Test Example from the KYST Manual: Unsymmetric Matrix of Similarity Measures: Regression: Descending

First we use descending isotone (monotone) regression for the relationship among data and model values:

```
simi = [ 9.30  0.57  6.10  2.00  1.50 ,
         1.00  8.50  5.50  3.30  4.00 ,
         2.10  5.30  7.30  3.90  1.10 ,
         5.00  6.20  1.60  8.90  2.80 ,
         1.30  4.10  1.00  2.50  8.80 ];
```

```
print "KYST MDS without initial values: Descending";
optn = [ "data"      "simi" ,
         "unsym"      ,
         "meth"      "kyst" ,
         "regres"    "desc" ,
         "pre-it"    3 ,
         "coord"    "rotat" ,
         "dimmax"    3 ,
         "dimmin"    1 ,
         "phis"      ,
         "norm"      ];
< gof,conf > = mds(sim, optn);
```

```
*****
NonMetric Multidimensional Scaling
*****
```

Similarity Input Data (Unsymmetric)

Number Rows of Matrix	5
Maximum Dimension	3
Minimum Dimension	1
Amount Input Information.	25
Number of Parameters.	15
Degrees of Freedom.	10
Stress Formula.	1
Diagonal	Included
Isotone Regression	Descending
Tie Treatment	Primary
Maximum Number Iterations	5000
TORSCA Preiterations.	3

Similarity Matrix: 1

1	9.3	0.57	6.1	2	1.5
---	-----	------	-----	---	-----

2	1	8.5	5.5	3.3	4
3	2.1	5.3	7.3	3.9	1.1
4	5	6.2	1.6	8.9	2.8
5	1.3	4.1	1	2.5	8.8

 Compute Kruskal-Young-Shepard-Torgerson KYST

 There are 25 data values, split into 1 lists.

Torgerson-Young Quasi-Nonmetric Procedure for Initial Configuration

Iteration	Stress
0	0.022638560
1	0.002207875
2	0.000459813
3	0.000153818

[note] file tmds1.inp, line 63: Maximum number of pre-iterations 3 reached.

The best initial configuration by Torgerson-Young quasi-nonmetric method has Stress=0.000153818 Formula 1

History of Iteration for 3 Dimensions

Iter	STRESS	SRAT	SRATAV	CAGRCL	COSAV	ACSAV	SFGR	STEP
0	0.010	0.800	0.800	0.000	0.000	0.000	0.0010	0.0002

Satisfactory Stress was reached after 0 iterations.

Final Configuration (Stress= 0.00989601 Formula 1)

	D_3_1	D_3_2	D_3_3
0_1	1.075123487	-0.513110454	-0.160950519
0_2	-0.696452481	0.652971078	-0.001235367
0_3	0.568985138	0.719528505	-0.156694064
0_4	0.008885202	-0.233080220	0.586641998
0_5	-0.956541346	-0.626308909	-0.267762048

Group	Count	Stress	Regression
1	25	0.00989601	Descending

History of Iteration for 2 Dimensions

Iter	STRESS	SRAT	SRATAV	CAGRCL	COSAV	ACSAV	SFGR	STEP
0	0.059	0.800	0.800	0.000	0.000	0.000	0.0039	0.0057
1	0.057	0.968	0.852	0.999	0.659	0.659	0.0037	0.0155
2	0.052	0.916	0.873	0.988	0.876	0.876	0.0031	0.0530
3	0.041	0.785	0.843	0.357	0.533	0.533	0.0014	0.1104
	0.060			-0.658				0.0110
4	0.039	0.966	0.882	0.757	0.681	0.681	0.0010	0.0291
5	0.037	0.948	0.903	0.216	0.374	0.374	0.0005	0.0476
	0.051			-0.940				0.0048
6	0.037	0.996	0.933	-0.490	-0.196	0.451	0.0002	0.0027
7	0.037	0.999	0.955	-0.283	-0.253	0.340	0.0002	0.0016
8	0.037	0.999	0.969	0.007	-0.081	0.120	0.0001	0.0012
9	0.037	1.000	0.979	0.219	0.117	0.185	0.0001	0.0011
10	0.037	1.000	0.986	-0.272	-0.140	0.242	0.0001	0.0007
11	0.037	1.000	0.991	-0.381	-0.299	0.334	0.0000	0.0003
12	0.037	1.000	0.994	0.111	-0.028	0.187	0.0000	0.0002
13	0.037	1.000	0.996	0.415	0.264	0.337	0.0000	0.0003
14	0.037	1.000	0.997	0.008	0.095	0.120	0.0000	0.0002
15	0.037	1.000	0.998	-0.704	-0.432	0.505	0.0000	0.0001
16	0.037	1.000	0.999	0.850	0.414	0.733	0.0000	0.0001
17	0.037	1.000	0.999	-0.496	-0.187	0.577	0.0000	0.0000

Minimum was achieved after 17 iterations.

Final Configuration (Stress= 0.0371116 Formula 1)

	D_2_1	D_2_2
0_1	1.147921385	-0.496658734
0_2	-0.646499738	0.672365556
0_3	0.649763151	0.672655794
0_4	-0.001631430	-0.354985561
0_5	-1.149553368	-0.493377055

Group Count Stress Regression

1 25 0.03711159 Descending

History of Iteration for 1 Dimensions

Iter	STRESS	SRAT	SRATAV	CAGRCL	COSAV	ACSAV	SFGR	STEP
------	--------	------	--------	--------	-------	-------	------	------

0	0.212	0.800	0.800	0.000	0.000	0.000	0.0109	0.0575
1	0.204	0.963	0.851	0.850	0.561	0.561	0.0006	0.1358
2	0.231	1.134	0.937	-0.946	-0.434	0.815	0.0187	0.0501
3	0.215	0.928	0.934	0.989	0.505	0.930	0.0110	0.0639
4	0.205	0.956	0.941	0.501	0.502	0.647	0.0029	0.1008
	0.213			-0.979				0.0101
5	0.205	0.997	0.959	0.997	0.829	0.878	0.0022	0.0267
6	0.204	0.997	0.972	-0.903	-0.314	0.895	0.0008	0.0094
	0.204			-0.977				0.0009
7	0.204	1.000	0.981	1.000	0.553	0.964	0.0006	0.0012
8	0.204	1.000	0.987	0.999	0.847	0.987	0.0004	0.0028
9	0.204	1.000	0.991	-0.649	-0.140	0.764	0.0001	0.0012
	0.204			-1.000				0.0001
10	0.204	1.000	0.994	1.000	0.612	0.920	0.0000	0.0002
11	0.204	1.000	0.996	1.000	0.868	0.973	0.0000	0.0004
	0.204			-1.000				0.0000
12	0.204	1.000	0.997	1.000	0.955	0.991	0.0000	0.0001
	0.204			-1.000				0.0000
13	0.204	1.000	0.998	1.000	0.985	0.997	0.0000	0.0000
	0.204			-0.990				0.0000
14	0.204	1.000	0.999	1.000	0.995	0.999	0.0000	0.0000
15	0.204	1.000	0.999	1.000	0.998	1.000	0.0000	0.0000

Minimum was achieved after 15 iterations.

Final Configuration (Stress= 0.203946 Formula 1)

D_1_1	
0_1	1.394282445
0_2	-0.663840798
0_3	0.746266448
0_4	-0.042636844
0_5	-1.434071249

Group	Count	Stress	Regression
1	25	0.20394609	Descending

4. Test Example from the KYST Manual: Unsymmetric Matrix of Similarity Measures: Regression: Third Order Polynomial

```
simi = [ 9.30  0.57  6.10  2.00  1.50 ,
         1.00  8.50  5.50  3.30  4.00 ,
         2.10  5.30  7.30  3.90  1.10 ,
```

```

5.00 6.20 1.60 8.90 2.80 ,
1.30 4.10 1.00 2.50 8.80 ];

```

```

print "KYST MDS without initial values: Polynomial Degree=3";
optn = [ "data"      "simi" ,
        "unsym"      ,
        "meth"      "kyst" ,
        "regres"    "poly" ,
        "poldeg"    3 ,
        "pre-it"    3 ,
        "coord"     "rotat" ,
        "dimmax"    3 ,
        "dimmin"    1 ,
        "phis"      ,
        "norm"      ];
< gof,conf > = mds(sim, optn);

```

```

*****
Metric Multidimensional Scaling
*****

```

```

Similarity Input Data (Unsymmetric)
Number Rows of Matrix . . . . . 5
Maximum Dimension . . . . . 3
Minimum Dimension . . . . . 1
Amount Input Information. . . . . 25
Number of Parameters. . . . . 15
Degrees of Freedom. . . . . 10
Stress Formula. . . . . 1
Diagonal . . . . . Included
Polynomial Regression Degree. . . . . 3
Maximum Number Iterations . . . . . 5000
TORSCA Preiterations. . . . . 3

```

```

*****
Compute Kruskal-Young-Shepard-Torgerson KYST
*****
There are 25 data values, split into 1 lists.

```

Torgerson-Young Quasi-Nonmetric Procedure for Initial Configuration

```

Iteration      Stress
              0 0.022638560

```

1 0.002207875
 2 0.000459813
 3 0.000153818

[note] file tmds1.inp, line 42: Maximum number of pre-iterations 3 reached.

The best initial configuration by Torgerson-Young quasi-nonmetric method has Stress=0.000153818 Formula 1

History of Iteration for 3 Dimensions

Iter	STRESS	SRAT	SRATAV	CAGRCL	COSAV	ACSAV	SFGR	STEP
0	0.169	0.800	0.800	0.000	0.000	0.000	0.0069	0.0293
1	0.163	0.968	0.852	0.974	0.643	0.643	0.0056	0.0776
2	0.153	0.939	0.880	0.738	0.706	0.706	0.0034	0.2093
3	0.155	1.008	0.921	-0.703	-0.224	0.704	0.0057	0.0997
4	0.147	0.948	0.930	-0.463	-0.382	0.545	0.0022	0.0464
5	0.146	0.998	0.952	-0.837	-0.682	0.738	0.0021	0.0153
6	0.146	0.995	0.966	0.934	0.384	0.867	0.0006	0.0152
7	0.146	1.000	0.977	-0.897	-0.462	0.887	0.0008	0.0048
8	0.146	0.999	0.985	0.983	0.492	0.950	0.0003	0.0054
9	0.146	1.000	0.990	-0.819	-0.374	0.864	0.0002	0.0018
10	0.146	1.000	0.993	0.401	0.138	0.559	0.0000	0.0012
11	0.146	1.000	0.995	0.574	0.426	0.569	0.0000	0.0016
12	0.146	1.000	0.997	-0.448	-0.151	0.489	0.0001	0.0008
13	0.146	1.000	0.998	-0.553	-0.416	0.531	0.0000	0.0003
14	0.146	1.000	0.999	-0.631	-0.558	0.597	0.0000	0.0001
15	0.146	1.000	0.999	0.901	0.405	0.798	0.0000	0.0001

Minimum was achieved after 15 iterations.

Final Configuration (Stress= 0.145597 Formula 1)

	D_3_1	D_3_2	D_3_3
0_1	0.966987925	-0.512572882	-0.077858169
0_2	-0.609811159	0.628542479	0.045316107
0_3	0.480826435	0.706684142	-0.399330276
0_4	-0.075197068	-0.128523217	0.908024094
0_5	-0.762806134	-0.694130522	-0.476151756

The regression coefficients start with the intercept and it is of no surprise that the coefficient of the order 3 term is negative indicating an descending behavior:

Group Count Stress Regression Coefficients

1 25 0.14559717 2.003 -0.206 0.030 -0.004

History of Iteration for 2 Dimensions

Iter	STRESS	SRAT	SRATAV	CAGRCL	COSAV	ACSAV	SFGR	STEP
0	0.209	0.800	0.800	0.000	0.000	0.000	0.0054	0.0281
1	0.206	0.986	0.858	0.929	0.613	0.613	0.0036	0.0714
2	0.203	0.983	0.898	0.149	0.307	0.307	0.0028	0.1094
3	0.205	1.012	0.934	-0.635	-0.315	0.524	0.0073	0.0547
4	0.200	0.973	0.947	0.532	0.244	0.529	0.0015	0.0535
5	0.200	1.002	0.965	-0.631	-0.333	0.596	0.0035	0.0232
6	0.199	0.994	0.975	0.775	0.398	0.714	0.0010	0.0260
7	0.199	1.000	0.983	-0.610	-0.267	0.645	0.0014	0.0109
8	0.199	0.999	0.988	0.742	0.399	0.709	0.0005	0.0119
9	0.199	1.000	0.992	-0.035	0.113	0.264	0.0005	0.0098
10	0.199	1.000	0.995	-0.483	-0.281	0.409	0.0005	0.0048
11	0.198	1.000	0.996	0.293	0.098	0.332	0.0002	0.0036
12	0.198	1.000	0.998	0.805	0.564	0.644	0.0002	0.0059
13	0.198	1.000	0.998	0.068	0.237	0.264	0.0002	0.0064
14	0.198	1.000	0.999	-0.851	-0.481	0.652	0.0005	0.0022
15	0.198	1.000	0.999	0.985	0.486	0.872	0.0003	0.0025

Minimum was achieved after 15 iterations.

Final Configuration (Stress= 0.198448 Formula 1)

	D_2_1	D_2_2
0_1	1.144281569	-0.497908299
0_2	-0.620555127	0.658039311
0_3	0.572111824	0.801728943
0_4	-0.004133515	-0.487920895
0_5	-1.091704751	-0.473939059

Group Count Stress Regression Coefficients

1 25 0.19844843 2.754 -0.894 0.176 -0.012

History of Iteration for 1 Dimensions

Iter	STRESS	SRAT	SRATAV	CAGRCL	COSAV	ACSAV	SFGR	STEP
------	--------	------	--------	--------	-------	-------	------	------

0	0.332	0.800	0.800	0.000	0.000	0.000	0.0078	0.0647
	0.330			-0.967				0.0065
1	0.332	0.998	0.861	1.000	0.660	0.660	0.0067	0.0175
2	0.330	0.996	0.904	0.998	0.883	0.883	0.0037	0.0593
	0.331			-0.989				0.0059
3	0.330	0.999	0.935	1.000	0.960	0.960	0.0027	0.0210
4	0.330	0.999	0.956	-0.929	-0.287	0.939	0.0009	0.0076
	0.330			-0.998				0.0008
5	0.330	1.000	0.970	1.000	0.563	0.979	0.0007	0.0010
6	0.330	1.000	0.980	1.000	0.851	0.993	0.0005	0.0024
7	0.330	1.000	0.987	0.995	0.946	0.994	0.0001	0.0071
	0.330			-0.999				0.0007
8	0.330	1.000	0.991	-0.430	0.038	0.622	0.0000	0.0004
	0.330			-0.992				0.0000
9	0.330	1.000	0.994	0.466	0.321	0.519	0.0000	0.0000
	0.330			-0.995				0.0000
10	0.330	1.000	0.996	0.953	0.738	0.805	0.0000	0.0000
	0.330			-1.000				0.0000
11	0.330	1.000	0.997	0.998	0.910	0.933	0.0000	0.0000
	0.330			-1.000				0.0000
12	0.330	1.000	0.998	1.000	0.969	0.977	0.0000	0.0000
	0.330			-1.000				0.0000
13	0.330	1.000	0.999	1.000	0.990	0.992	0.0000	0.0000
	0.330			-1.000				0.0000
14	0.330	1.000	0.999	1.000	0.996	0.997	0.0000	0.0000

Minimum was achieved after 14 iterations.

Final Configuration (Stress= 0.329676 Formula 1)

D_1_1	
0_1	1.452973688
0_2	-0.710018727
0_3	0.707880939
0_4	-0.080754068
0_5	-1.370081832

Group	Count	Stress	Regression	Coefficients
1	25	0.32967640	3.139	-1.212 0.223 -0.014

5. Example HANGUL by Yoshio Takane: 3-way Rectangular Data:
m=3, n=14

```
print "HANGUL: 3-way Rectangular Data: Nsub=3, Nobs=14";
```

```

n = 14; nw = 3; ndim = 3;
order = [ 24 31 8 42 21 91 25 55 85 15 50 51 27 30 39 26 2 88 87 29 68
          53 49 72 69 67 22 75 57 44 16 19 36 48 10 78 33 7 35 4 61 46
          83 38 70 54 77 74 60 28 3 11 80 64 66 40 43 52 79 56 76 47 71
          90 14 32 6 12 81 23 65 9 63 45 41 73 37 59 58 89 84 5 20 62
          18 13 34 17 1 82 86 ];
dis1 = [ 4 6 3 4 3 1 3 3 2 6 6 7 3 4 6 4 1 2 3 6 6 7 6 1 4 6 6 4 7 4 6 7 6 1 3
          1 4 4 2 4 1 1 6 7 4 6 6 4 7 4 6 6 7 6 3 6 1 4 6 7 7 8 6 2 4 6 6 7 7 3
          3 6 4 2 6 6 7 5 6 3 1 4 7 6 8 6 7 7 4 4 3 ];
dis2 = [ 2 3 1 6 7 1 6 3 5 5 6 5 2 3 6 6 1 2 4 6 3 7 8 3 6 5 6 7 5 6 6 7 6 2 7
          1 6 4 2 5 7 3 5 6 7 7 6 6 7 8 4 7 8 5 4 7 2 4 8 4 3 7 7 4 3 5 4 6 7 6
          2 7 7 2 7 5 6 6 3 6 2 5 6 2 7 3 7 6 5 8 4 ];
dis3 = [ 3 5 2 9 4 1 5 4 8 9 8 8 5 9 8 7 1 6 6 6 8 8 9 2 5 5 6 8 9 8 7 8 4 1 6
          1 9 7 6 8 2 2 7 8 9 6 6 3 8 7 6 5 6 4 3 8 7 6 6 6 7 9 8 2 8 8 6 7 6 4
          6 7 6 1 9 7 7 9 1 7 2 9 7 7 8 2 6 9 6 9 3 ];
dis1[order] = dis1; dis2[order] = dis2; dis3[order] = dis3;

/* get tensor diss[nw,n,n] */
real diss[nw,n,n];
diss[1,..] = vec2tri(dis1,n,"ssym"); diss[2,..] = vec2tri(dis2,n,"ssym");
diss[3,..] = vec2tri(dis3,n,"ssym");
print "Tensor diss=",diss;

rnam = [" GA NA DA LA MA BA SA AA JA CHA KA TA PA HA "];
wnam = [" NAOMI ISABELLE OLEX "];
list tnam[3];
tnam[1] = wnam; tnam[2] = tnam[3] = rnam;
diss = dimname(diss,tnam);
print "Tensor diss=",diss;

print "HANGUL: Symmetric: nsub=3, nobs=14, ndim=3";
optn = [ "data"      "diss" ,
          "symm"      ,
          "meth"      "mult" ,
          "model"     "dia" ,
          "regres"    "power" ,
          "ndim"      3 ,
          "ptab"      ,
          "pdis"      ,
          "pres"      ,
          "phis"      ] ;
options LS=80;
< gof,conf,wgt,res > = mds(diss,optn);

```

 3-Way Multidimensional Scaling

Dissimilarity Input Data (Symmetric)

Number Rows of Matrix	14
Dimension	3
Number Subjects / Replications.	3
Amount Input Information.	273
Number of Parameters.	51
Degrees of Freedom.	222
Maximum Number Iterations	50
Convergence Criterion for Main Iterations	0.05
Number of Constraint Equations.	0
Individual Metric Matrix.	DIAGONAL
Estimated Data Transformation Type.	POWER
Stimulus Variance Type.	CONSTANT
Subject Variance Type	SUBWISE
Assumed Error Distribution.	LogNormal
Maximum Number of Configuration Iterations.	1
Convergence Criterion for Configuration	0.000366367
Maximum Number of Metric Matrix Iterations.	1
Convergence Criterion for Metric Matrix	0.00109951
Standard Error Weight Estimates	Post-Hoc

 Compute Metric MULTISCALE by J. Ramsay

Zero Data: 0 Nonzero Data: 546

Initial Configuration Matrix

	DIM_1	DIM_2	DIM_3
GA	1.693392140	3.440379391	-0.058330375
NA	3.821119948	-0.865510991	-1.535791450
DA	1.242735081	2.824937623	2.057309005
LA	2.926946574	-0.817396710	0.605060613
MA	3.431472988	-0.370735784	-2.321494491
BA	-0.457316347	-1.568108691	2.953564288
SA	-2.857053380	-0.876447666	-2.282018660
AA	1.546868870	-2.013375035	1.268114706
JA	-0.740375144	-0.671116637	-2.832730182
CHA	-3.171367453	-0.345144311	-2.079653150
KA	-2.081242024	4.070858224	-0.393830538

TA -2.381454586 0.530835880 1.677753277
PA -0.755927749 -1.184727728 2.382583253
HA -2.217798916 -2.154447564 0.559463706

MainIter=0 ErrSS=34.7658 LogLik=-332.275 Std.Err=0.504672
Grad=3.37034

***** Main Iteration 1 *****

Configuration Iterations

Iter ErrorSS Penalty Grad

0 34.76577380 0.00000000 3.242322213

Line Search Convergence achieved after 4 Iterations.

0 20.19175731 0.00000000 0.808229728

Weight Matrix Iterations

Subj	Iter	ErrorSS	GradLgn
Line Search Convergence achieved after 3 Iterations.			
1	0	5.098514191	0.018974946
Line Search Convergence achieved after 3 Iterations.			
2	0	8.235164576	0.028990435
Line Search Convergence achieved after 4 Iterations.			
3	0	6.210575504	0.067967736

MainIter=1 ErrSS=18.5833 LogLik=-247.913 Std.Err=0.368973
Grad=0.781247

***** Main Iteration 17 *****

Configuration Iterations

Iter ErrorSS Penalty Grad

0 16.07777032 0.00000000 0.028864305

Line Search Convergence achieved after 3 Iterations.

0 16.07443345 0.00000000 0.016972150

Configuration matrix convergence achieved.

Weight Matrix Iterations

Subj Iter ErrorSS GradLgn

MainIter=17 ErrSS=16.0703 LogLik=-222.141 Std.Err=0.34312

Grad=0.0169858

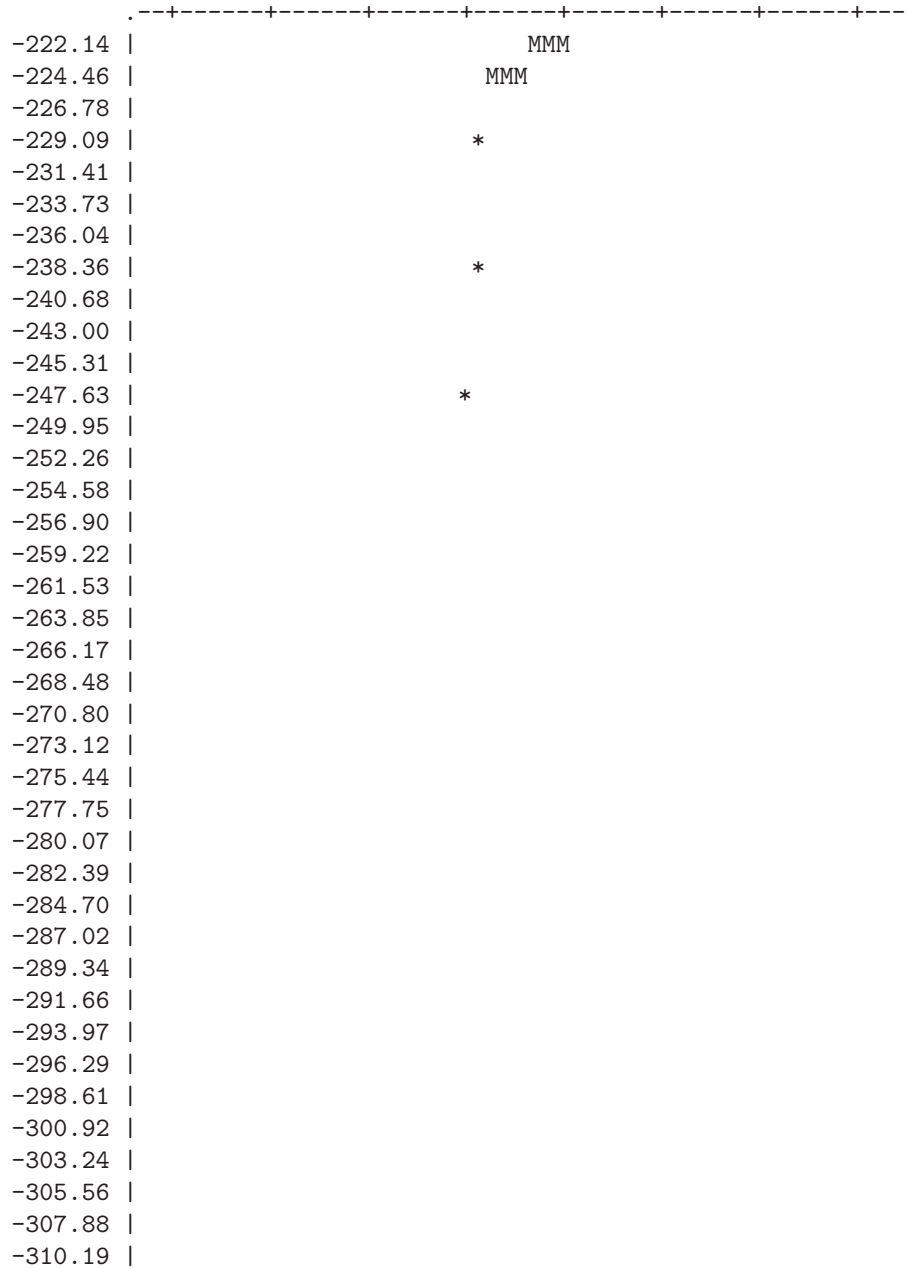
Main Convergence achieved after 17 Iterations.

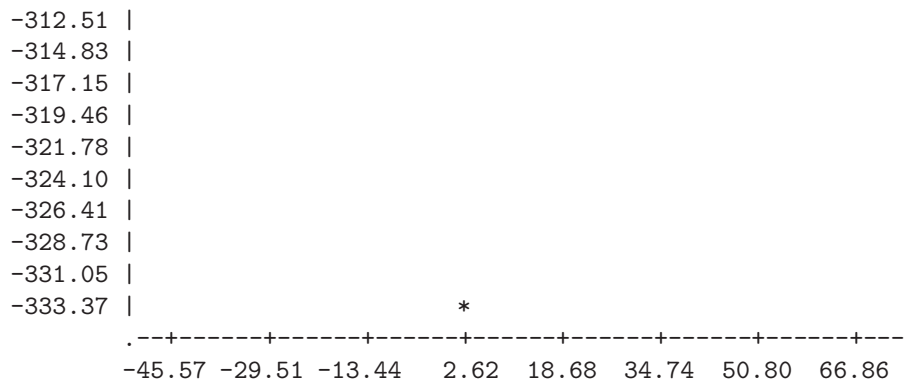
Post-Mortem Display of Iterations

Iter	LogLikel.	ErrorSSQ	Grad_Length
0	-332.275034	34.7657738	3.37034133
1	-247.912682	18.5832600	0.78124681
2	-237.995998	17.2037229	0.68795646
3	-228.132661	16.1328279	0.43250699
4	-224.694652	16.0185771	0.16987826
5	-224.111344	16.1412531	0.07203409
6	-223.947027	16.2305851	0.04191853
7	-223.834008	16.2993201	0.03925094
8	-223.718201	16.3456821	0.04228601
9	-223.562014	16.3497568	0.05768708
10	-223.325721	16.3119669	0.06698664
11	-222.986955	16.2402661	0.07156129
12	-222.696816	16.1705122	0.06266364
13	-222.459718	16.1037396	0.04617941
14	-222.320727	16.0801308	0.03924391
15	-222.224806	16.0631223	0.02864440
16	-222.170350	16.0777703	0.02346187

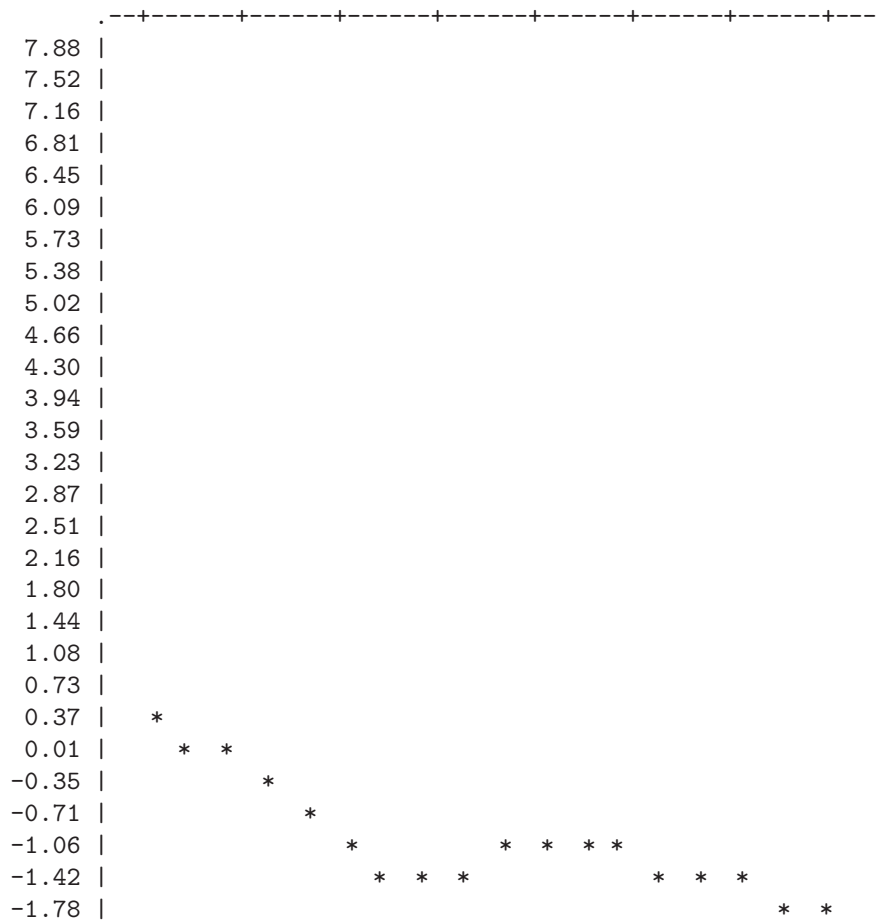
17 -222.140745 16.0703107 0.01698578

Log Likelihood Versus Iterations (Dimension=3)





Plot of LOG of Gradient Length vs. Iterations (Dim=3)



-----+-----+-----+-----+-----+-----+-----+-----+-----+-----
 1.00 3.48 5.96 8.44 10.92 13.40 15.88 18.35

 ML Results for 3 Dimensions

Log Likelihood.	-222.141
AIC Statistic	544.281
BIC Statistic	724.755
Unbiased Standard Error Estimate.	0.379642
Number of Parameters.	50
Number of Degrees of Freedom for Error.	223
Maximum Likelihood Standard Error Estimate.	0.34312

 ML Results for Zero Dimensions

Log Likelihood.	-397.547
AIC Statistic	801.093
BIC Statistic	811.922
Unbiased Standard Error Estimate.	0.572895
Number of Parameters.	3
Number of Degrees of Freedom for Error.	270

Chi Square for Comparing two Fits	350.812
Number of Degrees of Freedom for Chi Square	47
Probability of Exceeding this Chi Square.	0

Final Configuration Matrix

	DIM_1	DIM_2	DIM_3
GA	-5.833769549	42.95111349	17.49054187
NA	33.71451814	23.01910644	-46.62252275
DA	-6.972180399	32.30519044	26.21958755
LA	74.17208531	4.518121476	3.582671946
MA	40.00171750	38.78290758	-26.40205602
BA	14.43745091	-27.51251267	22.23081108
SA	-61.36680439	-19.85491655	-14.00618563
AA	32.53634008	-18.94987224	-12.58251102
JA	-34.72490670	-2.986183306	-33.73231834
CHA	-35.02008594	-20.98091483	-21.01765981
KA	-26.82689028	31.78583605	21.54301983
TA	-14.13338676	-18.90323856	28.52173339

PA -6.551859311 -31.25637806 24.62244759
 HA -3.432228613 -32.91825927 10.15244032
 The decimal point has been moved 1 places to the right.

Results in Polar Coordinate Form

	1	2	3
GA	46.741310	98.000000	108.000000
NA	61.969409	34.000000	-54.000000
DA	42.186531	102.000000	105.000000
LA	74.395882	3.0000000	3.0000000
MA	61.654845	44.000000	-33.000000
BA	38.204546	-62.000000	57.000000
SA	66.002088	198.00000	193.00000
AA	39.699253	-30.000000	-21.000000
JA	48.503667	185.00000	224.00000
CHA	45.916742	211.00000	211.00000
KA	46.841468	130.00000	141.00000
TA	37.021269	233.00000	116.00000
PA	40.325587	258.00000	105.00000
HA	34.618839	264.00000	109.00000

First Value is Distance from the Origin
 Other Values are Angles in Degrees from First Dimension

 Standard Deviations and Variances for each Dimension

Dim	Std.Dev.	Variance	Percent
1	34.60001437	1197.160994	47
2	27.16411058	737.8889034	29
3	24.33720052	592.2993292	23

Interpoint Distances

	GA	NA	DA	LA
GA	0	77	13	89
NA	77	0	83	67
DA	13	83	0	88
LA	89	67	88	0
MA	63	26	70	56
BA	73	87	63	70
SA	89	109	85	138

AA	78	54	75	50
JA	74	74	74	115
CHA	80	85	76	114
KA	24	91	20	106
TA	63	98	51	94
PA	74	98	63	90
HA	76	87	67	86

.....

Final Weight Matrix

	DIM_1	DIM_2	DIM_3
NAOMI	0.412642095	1.155887660	1.222149835
ISABELLE	1.218159780	1.158094466	0.418215205
OLEX	1.160933994	0.567936658	1.153117607

Results in Polar Coordinate Form

	1	2	3
NAOMI	1.7320508	70.000000	45.000000
ISABELLE	1.7320508	44.000000	43.000000
OLEX	1.7320508	26.000000	0.000000

First Value is Distance from the Origin

Other Values are Angles in Degrees from First Dimension

 Post-Hoc Standard Error Weight Estimates

	Input Order		Size Order
1	GA 0.0000000	1	GA 0.0000000
2	NA 0.61133448	4	LA 0.16585465
3	DA 2.29960410	5	MA 0.25344875
4	LA 0.16585465	2	NA 0.61133448
5	MA 0.25344875	13	PA 0.64146629
6	BA 1.26767980	11	KA 0.81903743
7	SA 1.66273222	14	HA 0.87274233
8	AA 1.25955433	9	JA 1.06895864
9	JA 1.06895864	8	AA 1.25955433
10	CHA 1.49133855	6	BA 1.26767980
11	KA 0.81903743	10	CHA 1.49133855
12	TA 2.00985566	7	SA 1.66273222
13	PA 0.64146629	12	TA 2.00985566
14	HA 0.87274233	3	DA 2.29960410

 Final Regression Coefficient and Exponent Estimates

Subject	Regression Coefficient	Exponent	Reciprocal	Subject	Exponent by Size
1 NAOMI	1.40680746	0.93303742	1.07176838	1 NAOMI	0.93303742
2ISABELLE	0.72030562	1.31213620	0.76211601	3 OLEX	0.99164164
3 OLEX	0.98684407	0.99164164	1.00842881	2ISABELLE	1.31213620

Mean= 1.07894 Standard Deviation= 0.20407

 Within-Subj. Std.Error Estimates and Multiple Correlations

Subj	Standard Error			Multiple Correlation			
	Unordered	Subj	Ordered	Subj	Unordered	Subj	Ordered
1	0.22	1	0.22	1	0.91	2	0.67
2	0.45	3	0.32	2	0.67	3	0.75
3	0.32	2	0.45	3	0.75	1	0.91

 Asympt. Standard Errors of Estimate of Coordinates

1	GA	-0.5834	4.2951	1.7491
		0.7183	0.8379	0.6427

Correlation Matrix 1 for Coordinate Estimates

	DIM_1	DIM_2	DIM_3
DIM_1	1.000000000	-0.024978736	0.440441259
DIM_2	-0.024978736	1.000000000	-0.092418119
DIM_3	0.440441259	-0.092418119	1.000000000

2	NA	3.3715	2.3019	-4.6623
		0.4957	0.7825	0.4466

Correlation Matrix 2 for Coordinate Estimates

	DIM_1	DIM_2	DIM_3
--	-------	-------	-------

DIM_1	1.000000000	0.033762208	-0.100446586
DIM_2	0.033762208	1.000000000	-0.455694562
DIM_3	-0.100446586	-0.455694562	1.000000000

3	DA	-0.6972	3.2305	2.6220
		0.4882	0.5092	0.6462

Correlation Matrix 3 for Coordinate Estimates

	DIM_1	DIM_2	DIM_3
DIM_1	1.000000000	0.133052899	0.175968019
DIM_2	0.133052899	1.000000000	0.077459569
DIM_3	0.175968019	0.077459569	1.000000000

4	LA	7.4172	0.4518	0.3583
		0.5384	0.5615	0.5177

Correlation Matrix 4 for Coordinate Estimates

	DIM_1	DIM_2	DIM_3
DIM_1	1.000000000	-0.485018869	-0.046880810
DIM_2	-0.485018869	1.000000000	-0.209008714
DIM_3	-0.046880810	-0.209008714	1.000000000

5	MA	4.0002	3.8783	-2.6402
		0.5040	0.5151	0.4546

Correlation Matrix 5 for Coordinate Estimates

	DIM_1	DIM_2	DIM_3
DIM_1	1.000000000	0.491034736	-0.057189755
DIM_2	0.491034736	1.000000000	-0.071323172
DIM_3	-0.057189755	-0.071323172	1.000000000

6	BA	1.4437	-2.7513	2.2231
		0.9316	0.5191	0.8535

Correlation Matrix 6 for Coordinate Estimates

	DIM_1	DIM_2	DIM_3
DIM_1	1.000000000	-0.588478790	0.025758511
DIM_2	-0.588478790	1.000000000	-0.107072269
DIM_3	0.025758511	-0.107072269	1.000000000

7	SA	-6.1367	-1.9855	-1.4006
		0.7397	0.5875	0.9220

Correlation Matrix 7 for Coordinate Estimates

	DIM_1	DIM_2	DIM_3
DIM_1	1.000000000	-0.304544151	-0.114603685
DIM_2	-0.304544151	1.000000000	-0.361201975
DIM_3	-0.114603685	-0.361201975	1.000000000

8	AA	3.2536	-1.8950	-1.2583
		0.6351	0.7670	0.6686

Correlation Matrix 8 for Coordinate Estimates

	DIM_1	DIM_2	DIM_3
DIM_1	1.000000000	-0.063057167	-0.127590439
DIM_2	-0.063057167	1.000000000	0.671252254
DIM_3	-0.127590439	0.671252254	1.000000000

9	JA	-3.4725	-0.2986	-3.3732
		0.5475	0.5658	0.5126

Correlation Matrix 9 for Coordinate Estimates

	DIM_1	DIM_2	DIM_3
DIM_1	1.000000000	0.513133620	0.456933319
DIM_2	0.513133620	1.000000000	0.781066209
DIM_3	0.456933319	0.781066209	1.000000000

10	CHA	-3.5020	-2.0981	-2.1018
		0.4702	0.7437	0.5956

Correlation Matrix 10 for Coordinate Estimates

	DIM_1	DIM_2	DIM_3
DIM_1	1.000000000	-0.264506346	-0.196169208
DIM_2	-0.264506346	1.000000000	0.319587558
DIM_3	-0.196169208	0.319587558	1.000000000

11	KA	-2.6827	3.1786	2.1543
		0.6329	0.8756	0.7605

Correlation Matrix 11 for Coordinate Estimates

	DIM_1	DIM_2	DIM_3	
DIM_1	1.000000000	-0.080332951	0.401870991	
DIM_2	-0.080332951	1.000000000	0.213916668	
DIM_3	0.401870991	0.213916668	1.000000000	
12	TA	-1.4133	-1.8903	2.8522
		0.5556	0.6714	0.5545

Correlation Matrix 12 for Coordinate Estimates

	DIM_1	DIM_2	DIM_3	
DIM_1	1.000000000	0.139738633	0.404038865	
DIM_2	0.139738633	1.000000000	-0.109471051	
DIM_3	0.404038865	-0.109471051	1.000000000	
13	PA	-0.6552	-3.1256	2.4622
		0.5078	0.5252	0.7352

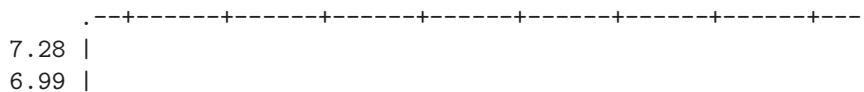
Correlation Matrix 13 for Coordinate Estimates

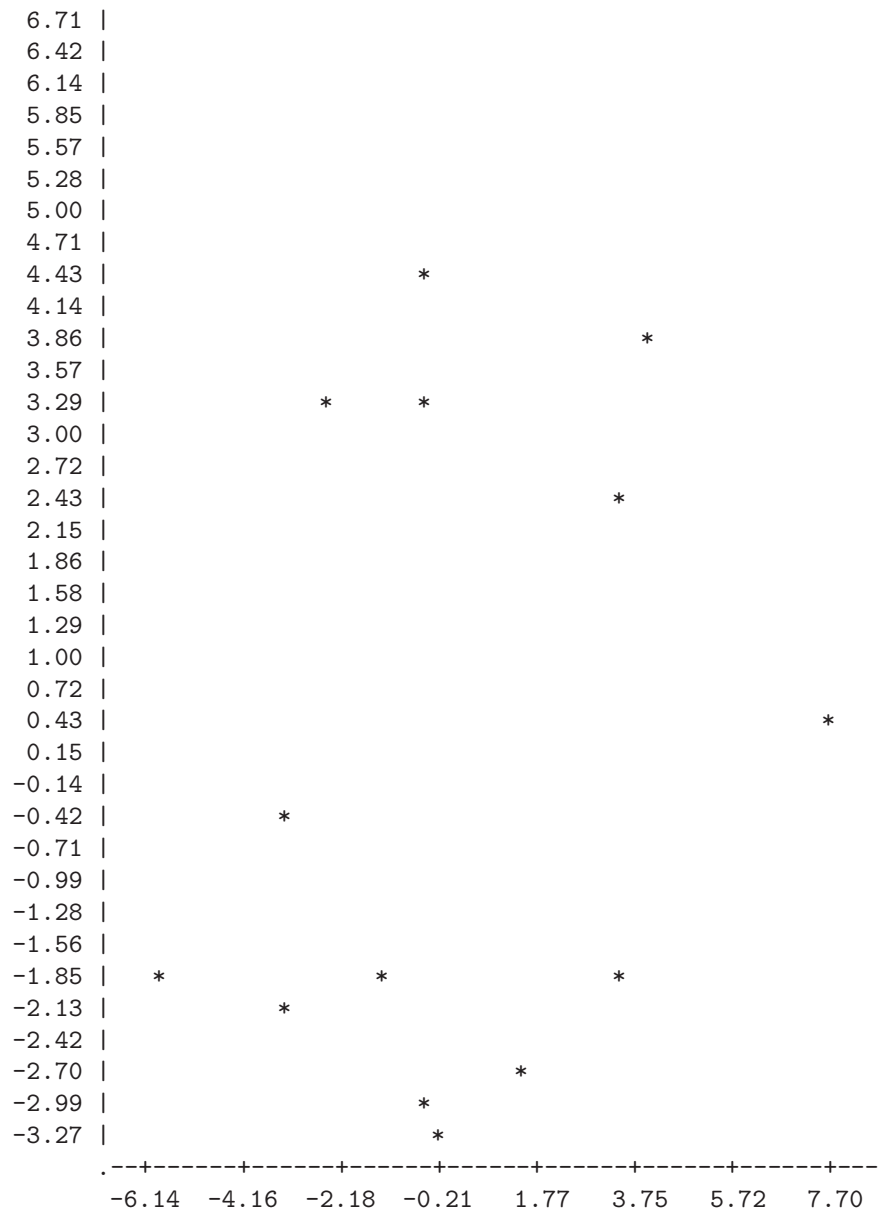
	DIM_1	DIM_2	DIM_3	
DIM_1	1.000000000	0.336710058	-0.014465145	
DIM_2	0.336710058	1.000000000	-0.240615577	
DIM_3	-0.014465145	-0.240615577	1.000000000	
14	HA	-0.3432	-3.2918	1.0152
		0.4934	0.5487	0.5469

Correlation Matrix 14 for Coordinate Estimates

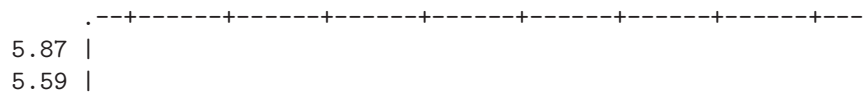
	DIM_1	DIM_2	DIM_3
DIM_1	1.000000000	0.505301215	0.531299385
DIM_2	0.505301215	1.000000000	0.877935810
DIM_3	0.531299385	0.877935810	1.000000000

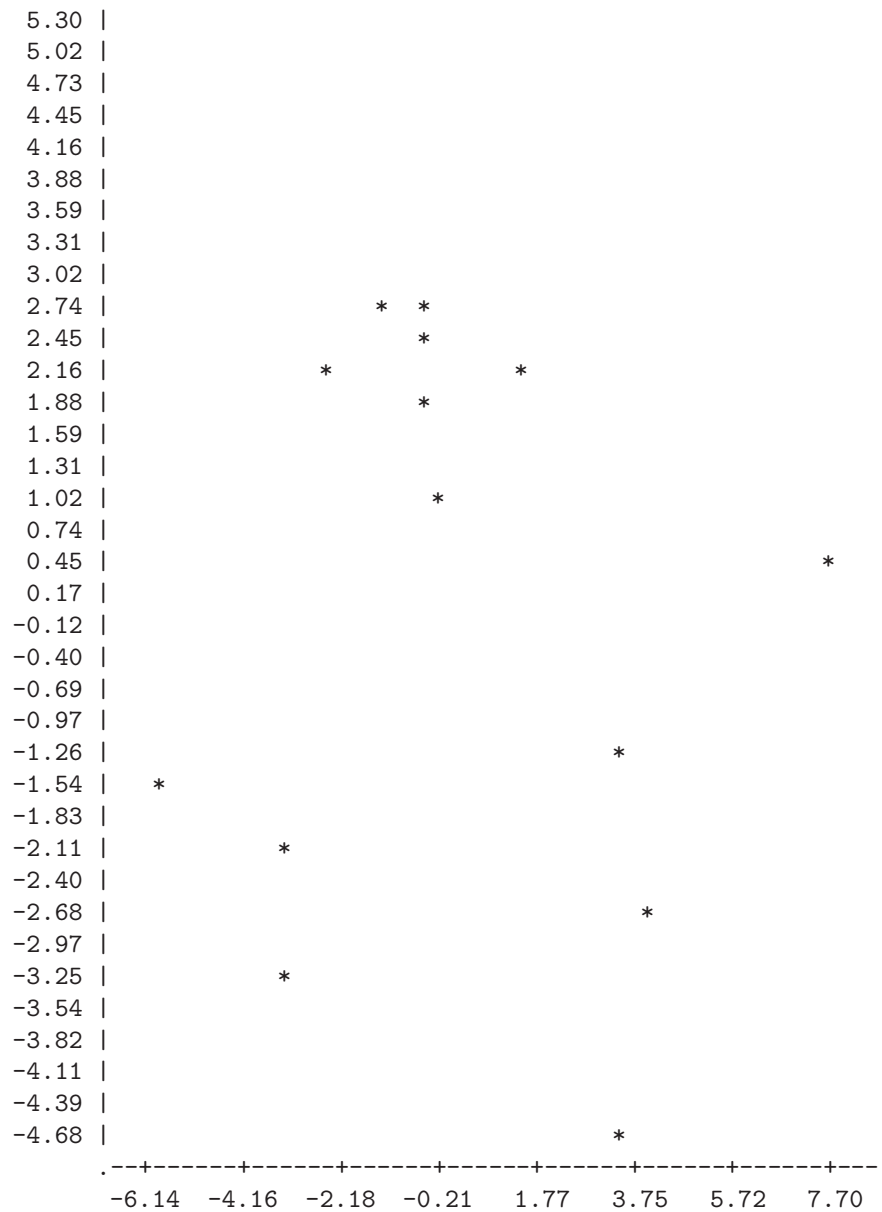
Configuration: Dimension 2 (Y-Axis) vs. Dimension 1 (X-Axis)



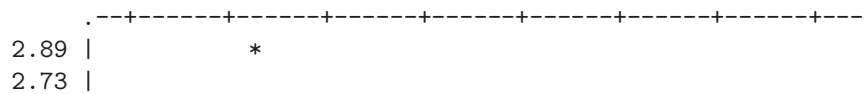


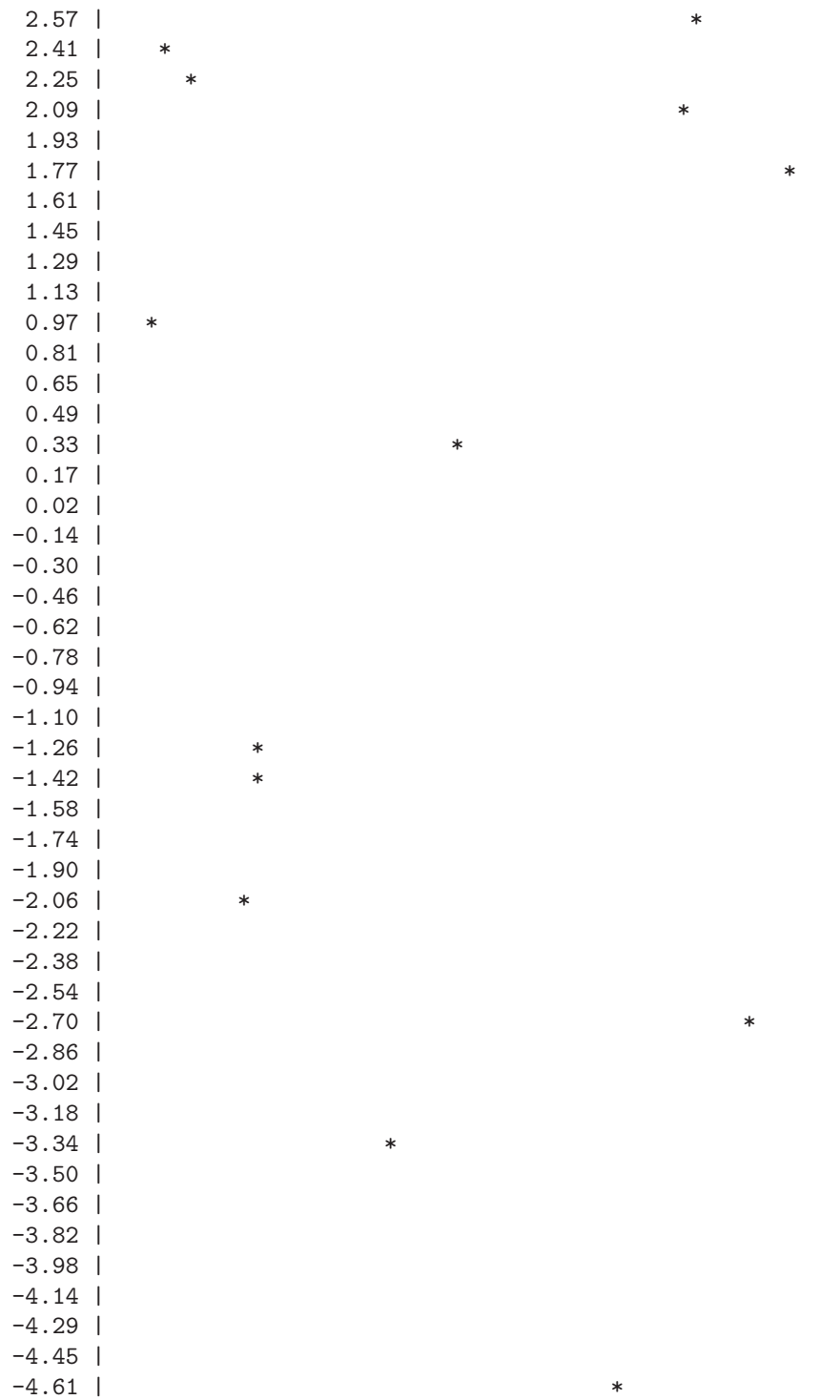
Configuration: Dimension 3 (Y-Axis) vs. Dimension 1 (X-Axis)





Configuration: Dimension 3 (Y-Axis) vs. Dimension 2 (X-Axis)





-----+-----+-----+-----+-----+-----+-----+-----+-----+-----
 -3.29 -2.19 -1.08 0.03 1.13 2.24 3.35 4.45

Transformed Observations: Subject=1

	GA	NA	DA	LA
GA	0.000000000	5.128367782	1.406807460	5.128367782
NA	5.128367782	0.000000000	7.486501175	5.128367782
DA	1.406807460	7.486501175	0.000000000	7.486501175
LA	5.128367782	5.128367782	7.486501175	0.000000000
MA	5.128367782	3.921088520	7.486501175	3.921088520
BA	7.486501175	8.644557291	7.486501175	5.128367782
SA	7.486501175	8.644557291	9.791549267	8.644557291
AA	7.486501175	3.921088520	5.128367782	3.921088520
JA	7.486501175	5.128367782	7.486501175	7.486501175
CHA	8.644557291	8.644557291	7.486501175	7.486501175
KA	1.406807460	9.791549267	1.406807460	7.486501175
TA	8.644557291	8.644557291	7.486501175	6.315385005
PA	7.486501175	7.486501175	5.128367782	5.128367782
HA	7.486501175	8.644557291	8.644557291	5.128367782

.....
 Smallest Value: 1.40681 Largest Value: 9.79155

Interpoint Distances: Subject=1

	GA	NA	DA	LA
GA	0.000000000	7.158159131	1.370558004	6.191635096
NA	7.158159131	0.000000000	7.795151562	5.891682281
DA	1.370558004	7.795151562	0.000000000	5.951115483
LA	6.191635096	5.891682281	5.951115483	0.000000000
MA	5.206060788	2.591533808	6.026122181	4.956083155
BA	7.045076335	8.625782950	6.027053099	5.077400153
SA	7.674641926	7.734798475	7.282667820	8.502045660
AA	7.166111207	5.372933335	6.794128139	3.738176556
JA	7.077124791	4.939050764	7.170939395	7.462352230
CHA	7.589068483	6.458338546	7.277167683	7.321478936
KA	1.700929113	7.801900058	1.259435926	6.758443997
TA	6.201400534	9.087634037	5.057124107	6.209752037
PA	7.330885611	9.269960481	6.250776957	6.274938090
HA	7.496727933	8.242553984	6.617793875	5.896113597

.....
 Smallest Value: 1.25944 Largest Value: 9.26996

Normalized Residuals: Subject=1

	MA	BA	SA	AA
GA	-0.067030618	0.270923841	-0.110647805	0.194985653
NA	1.846142233	0.009692450	0.495731186	-1.404289434
DA	0.967375305	0.966686685	1.319666588	-1.253906046
LA	-1.044269497	0.044526847	0.074105732	0.212964481
MA	0.000000000	-0.460180256	0.137649537	-0.595626465
BA	-0.460180256	0.000000000	-1.756529498	0.173533385
SA	0.137649537	-1.756529498	0.000000000	-0.326683485
AA	-0.595626465	0.173533385	-0.326683485	0.000000000
JA	-0.741271493	1.074014716	-0.535849169	2.020291872
CHA	0.073331919	-0.136792760	-0.858941556	1.037428300
KA	0.787188369	1.400725162	-1.085591432	0.943633307
TA	0.049187159	-1.533094294	1.696078236	0.132744744
PA	-0.834288953	0.320711097	1.638671557	0.514433155
HA	-0.490682645	-0.832249088	-2.180979586	0.622017989

.....

Smallest Value: -2.42579 Largest Value: 2.43163

Quantiles of Normalized Residuals: Subject=1

	GA	NA	DA	LA
GA	0.000000000	-1.359962536	0.054375453	-0.744341114
NA	-1.359962536	0.000000000	-0.332563025	-0.574739567
DA	0.054375453	-0.332563025	0.000000000	1.027144882
LA	-0.744341114	-0.574739567	1.027144882	0.000000000
MA	-0.247313727	1.844177266	0.938731970	-0.981979846
BA	0.390753455	-0.191527695	0.897170710	-0.136356872
SA	-0.275495595	0.511531310	1.294223527	-0.054375453
AA	0.275495595	-1.294223527	-1.233639904	0.332563025
JA	0.361503163	0.163876553	0.247313727	-0.163876553
CHA	0.640341274	1.233639904	0.081626883	0.027173016
KA	-0.780818419	0.981979846	0.480696247	0.450314414
TA	1.432159890	-0.361503163	1.712054734	-0.027173016
PA	1.0101e-007	-0.938731970	-0.857103039	-0.897170710
HA	-0.219332424	0.303903190	1.177268879	-0.607212923

.....

Smallest Value: -2.29533 Largest Value: 2.29533

3.13 Function selc

`< ntxtgen, ntxtforb > = selc(inides, forbid, nlev, optn)`

Purpose: Sequential elimination of level combinations algorithm: a method using the cross over and mutation operations of a genetic algorithm for finding nearly optimal experimental designs. For a given data set containing categorical data describing the level combinations for experiments with an outcome value y and a matrix of forbidden designs a new matrix of promising designs is computed. The new designs then must be used in experiments and corresponding outcome values determined. Depending on the outcome of the experiments the designs are then either added to the new initial design or used in adding new rows to the forbidden array and the computation is repeated.

Input: inides this is a $N \times n + 1$ matrix containing the integer level measurements (levels) of n categorical effects x_j in its first columns and an integer outcome y in its last column which can be positive or negative.

forbid this is a $M \times n$ matrix containing the M forbidden level combinations of the n effects.

nlev this is an n vector of positive integers specifying the upper most level for each effect. (Specifying this information is necessary since the data may have unobserved levels.)

optn

1. amount of printed output (=0: no output)
2. P the integer number of offsprings, i.e. the number promising level combinations to be computed which is the number of rows of the output argument **ntxtdes**. P must be a positive integer, default is 10.
3. s the integer strength applied to the forbidden array. s should be a positive integer, default is 2.
4. o the order applied to the forbidden array, default is 2.
5. should be either 1 for maximization (default) or 0 for minimization. (Depends on the orientation of the values of the outcome y .)
6. specifies the seed value for the random generator (default is time of day).

Output: ntxtdes This is an $P \times n$ matrix with the P promising level combinations found by the algorithm. Note, P is specified by **optn**[2].

ntxtforb During the computation the input forbidden array is extended by additional rows. This output argument shows the input forbidden array in the first rows and for the last rows the newly added forbidden patterns as used in the algorithm.

- Restrictions:**
1. The level measurements of the data `inides` and `forbid` array must be integers in $[1, K_j]$ for the effect j .
 2. The outcome variable y may consist of integers which can be positive or negative.

Relationships:

- Examples:**
1. Small example without significant interactions: Note, that level 5 in effect 1 is not contained in the data of the initial design.

```

options NOECHO;
ides = [
%inc "..\tdata\selc.dat";
];
options ECHO;

forbid = [ 3 10 3, 1 23 10, 1 23 23, 1 25 10,
          2 21 57, 2 23 57, 2 29 32, 2 29 57,
          2 30 57, 2 32 57, 2 33 57, 2 34 17,
          2 34 32, 2 34 34, 2 34 36, 2 34 37,
          2 34 45, 2 34 54, 2 34 56, 2 34 57,
          2 34 179, 3 23 10, 3 23 23, 3 25 21,
          3 25 23, 3 25 24, 4 21 57, 4 23 10,
          4 23 21, 4 23 29, 4 23 139, 4 23 171,
          4 23 185, 4 23 214, 4 25 21, 4 25 24,
          4 25 52, 4 25 125, 4 25 139, 4 25 171,
          4 25 185, 4 25 214, 4 25 222, 4 25 224,
          4 25 229, 4 29 32, 4 29 57, 4 30 57,
          4 33 57, 4 34 32, 4 34 34, 4 34 36,
          4 34 37, 4 34 45, 4 34 54, 4 34 56,
          4 34 57, 4 34 179, 5 18 119, 5 18 136,
          5 18 148, 5 18 153, 5 18 156, 5 18 181,
          5 18 182, 5 18 195, 5 18 197, 5 19 148,
          5 20 148, 5 20 181, 5 20 182 ];

inides = shape(ides,.,4);
print "nrow=",nrow(inides);
nlev = [ 5 34 241 ];

print "Option like MATLAB";
optn = [ 2 , /* ipri */
        10 , /* noff */
        2 , /* istr */
        2 , /* ordr */
        1 , /* imax */

```

```

        123 ]; /* seed */
optn[10] = 1;
< nxtdes,nxtforb > = selc(inides,forbid,nlev,optn);

```

```

*****
Sequential Elimination of Level Combinations (Maximization)
*****

```

Number of Observations	173
Rows of Forbidden Array.	71
Number Offspring	10
Strength of Forbidden Array	2
Order of Forbidden Array	2

Input: Level Numbers for Effects

	1
Eff_1	5
Eff_2	34
Eff_3	241

Frequencies of Effect Levels in Initial Design

1	1	26	3	1	11
	2	24		3	6
	3	69		6	9
	4	54		8	12
2	1	10		9	7
	2	8		10	4
	3	14		11	4
	4	6		13	12
	5	6		14	4
	6	13		20	10
	7	8		22	2
	8	8		27	7
	9	8		28	12
	10	9		30	10
	12	8		32	2
	13	9		34	7
	14	10		35	7
	15	11		37	4
	16	5		40	7
	17	2		46	15
	22	11		54	1
	23	4		58	3
	24	8		172	9
	25	1		227	8
	27	3			
	28	11			

There are 4 observations added to the forbidden array.

Output: Next Design

Dense Matrix (10 by 3)

	Eff_1	Eff_2	Eff_3
1	1	6	226
2	2	18	30
3	2	6	6
4	1	32	28
5	3	6	127

6	3	22	64
7	4	26	46
8	1	6	89
9	2	15	158
10	3	24	40

New Forbidden Array

Dense Matrix (75 by 3)

	1	2	3
1	3	10	3
2	1	23	10
3	1	23	23
4	1	25	10
5	2	21	57
6	2	23	57
7	2	29	32
8	2	29	57
9	2	30	57
10	2	32	57
11	2	33	57
12	2	34	17
13	2	34	32
14	2	34	34
15	2	34	36
16	2	34	37
17	2	34	45
18	2	34	54
19	2	34	56
20	2	34	57
21	2	34	179
22	3	23	10
23	3	23	23
24	3	25	21
25	3	25	23
26	3	25	24
27	4	21	57
28	4	23	10
29	4	23	21
30	4	23	29
31	4	23	139
32	4	23	171

33	4	23	185
34	4	23	214
35	4	25	21
36	4	25	24
37	4	25	52
38	4	25	125
39	4	25	139
40	4	25	171
41	4	25	185
42	4	25	214
43	4	25	222
44	4	25	224
45	4	25	229
46	4	29	32
47	4	29	57
48	4	30	57
49	4	33	57
50	4	34	32

	1	2	3
51	4	34	34
52	4	34	36
53	4	34	37
54	4	34	45
55	4	34	54
56	4	34	56
57	4	34	57
58	4	34	179
59	5	18	119
60	5	18	136
61	5	18	148
62	5	18	153
63	5	18	156
64	5	18	181
65	5	18	182
66	5	18	195
67	5	18	197
68	5	19	148
69	5	20	148
70	5	20	181
71	5	20	182
72	1	13	9
73	3	8	3
74	3	10	3

```

print "Option like SAS/IML version";
optn = [ 2 , /* ipri */
        5 , /* noff */
        10 , /* istr */
        2 , /* ordr */
        1 , /* imax */
        1 ]; /* seed */
nxtdes = selc(inides,forbid,nlev,optn);
print "Nextdes=",nxtdes;

```

2. Example containing significant interactions:

```

print "Johnson, Mandal, Ding: JSS 317: Revised Example 2";
options NOECHO;
ides = [
%inc "..\tdata\selc2.dat";
];
options ECHO;

forbid = .;
inides2 = shape(ides,.,5);
print "nrow=",nrow(inides2);
nlev = [ 11 11 11 11 ];

optn = [ 2 , /* ipri */
        5 , /* noff */
        2 , /* istr */
        2 , /* ordr */
        1 , /* imax */
        1 ]; /* seed */
optn[10] = 1;
< nxtdes,nxtforb > = selc(inides2,forbid,nlev,optn);
print "Nextdes=",nxtdes;
print "NextForb=",nxtforb;

```

```

*****
Sequential Elimination of Level Combinations (Maximization)
*****

```

```

Number of Observations . . . . . 242
Rows of Forbidden Array. . . . . 0
Number Offspring . . . . . 5

```

Strength of Forbidden Array 2
 Order of Forbidden Array 2

Input: Level Numbers for Effects

1
 Eff_1 11
 Eff_2 11
 Eff_3 11
 Eff_4 11

Frequencies of Effect Levels in Initial Design

1	1	22	3	1	22
	2	22		2	22
	3	22		3	22
	4	22		4	22
	5	22		5	22
	6	22		6	22
	7	22		7	22
	8	22		8	22
	9	22		9	22
	10	22		10	22
	11	22		11	22
2	1	22	4	1	22
	2	22		2	22
	3	22		3	22
	4	22		4	22
	5	22		5	22
	6	22		6	22
	7	22		7	22
	8	22		8	22
	9	22		9	22
	10	22		10	22
	11	22		11	22

There are 2 observations added to the forbidden array.

Output: Next Design

Dense Matrix (5 by 4)

	Eff_1	Eff_2	Eff_3	Eff_4
1	10	11	11	5
2	8	8	8	1
3	3	8	11	10
4	11	3	11	6
5	9	10	11	3

New Forbidden Array

Dense Matrix (2 by 4)

	1	2	3	4
1	4	2	3	3
2	7	2	4	2

3.14 Function urd1out

```
< effrep,outrep,cordat > = urd1out(X,y<,optn>)
```

Purpose: The function judges significant effects in unreplicated 2^k and 2^{k-p} factorial designs. The method makes it possible to detect a single outlier with the method by Daniel (1960).

Input: X is an $N \times n$, $N > n$, matrix of N designs for n effects coded in integers.

y is an N vector of real response values.

optn

Output: **effrep** a table of effects indicating which is found significant

outrep a table describing the outlier analysis

cordat a table of the original and corrected response data indicating which of the y is found an outlier

Restrictions: 1. The input data X and y may not contain any missing values or string data.

2. The number of rows of matrix X and vector y must be the same.

Relationships:

Examples: 1. Example 1 of submission:

```
nobs = 16; neff = 15;
xdat = cons(nobs,neff,.);
xrow = cons(1,neff,.);
i = 1;
for (d = -1; d <= 1; d+=2)
for (c = -1; c <= 1; c+=2)
for (b = -1; b <= 1; b+=2)
for (a = -1; a <= 1; a+=2) {
    xrow[1] = a; xrow[2] = b; xrow[3] = c; xrow[4] = d;
    xrow[5] = a*b; xrow[6] = a*c; xrow[7] = a*d;
    xrow[8] = b*c; xrow[9] = b*d; xrow[10] = c*d;
    xrow[11] = a*b*c; xrow[12] = a*b*d; xrow[13] = a*c*d;
    xrow[14] = b*c*d; xrow[15] = a*b*c*d;
    xdat[i,] = xrow; i++;
}
cnam = [" a b c d ab ac ad bc bd cd abc abd acd bcd abcd "];
xdat = cname(xdat,cnam);
```

```

print "Example1 of Submission: nobs=16=2^4, neff=11";
y1 = [ 1.68 1.98 3.28 3.44 4.98 5.70 9.97 9.07 2.07
      2.44 4.09 4.53 7.77 9.43 11.75 16.3 ];
y1 = log10(y1); /* print y1; */
optn = [ 2 ]; /* ipri */
< effrep,outrep,cordat > = urdlout(xdat,y1,optn);

```

```

*****
Analysis of Unreplicated 2^k and 2^(k-p) Designs (Lawson, 2007)
*****

```

```

Number of Observations . . . . . 16
Number of Effects. . . . . 15

```

Input Design Matrix

	a	b	c	d	ab	ac	ad	bc	bd
1	-1.000	-1.000	-1.000	-1.000	1.000	1.000	1.000	1.000	1.000
2	1.000	-1.000	-1.000	-1.000	-1.000	-1.000	-1.000	1.000	1.000
3	-1.000	1.000	-1.000	-1.000	-1.000	1.000	1.000	-1.000	-1.000
4	1.000	1.000	-1.000	-1.000	1.000	-1.000	-1.000	-1.000	-1.000
5	-1.000	-1.000	1.000	-1.000	1.000	-1.000	1.000	-1.000	1.000
6	1.000	-1.000	1.000	-1.000	-1.000	1.000	-1.000	-1.000	1.000
7	-1.000	1.000	1.000	-1.000	-1.000	-1.000	1.000	1.000	-1.000
8	1.000	1.000	1.000	-1.000	1.000	1.000	-1.000	1.000	-1.000
9	-1.000	-1.000	-1.000	1.000	1.000	1.000	-1.000	1.000	-1.000
10	1.000	-1.000	-1.000	1.000	-1.000	-1.000	1.000	1.000	-1.000
11	-1.000	1.000	-1.000	1.000	-1.000	1.000	-1.000	-1.000	1.000
12	1.000	1.000	-1.000	1.000	1.000	-1.000	1.000	-1.000	1.000
13	-1.000	-1.000	1.000	1.000	1.000	-1.000	-1.000	-1.000	-1.000
14	1.000	-1.000	1.000	1.000	-1.000	1.000	1.000	-1.000	-1.000
15	-1.000	1.000	1.000	1.000	-1.000	-1.000	-1.000	1.000	1.000
16	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000

Input Design Matrix

	cd	abc	abd	acd	bcd	abcd
1	1.000	-1.000	-1.000	-1.000	-1.000	1.000
2	1.000	1.000	1.000	1.000	-1.000	-1.000
3	1.000	1.000	1.000	-1.000	1.000	-1.000
4	1.000	-1.000	-1.000	1.000	1.000	1.000
5	-1.000	1.000	-1.000	1.000	1.000	-1.000
6	-1.000	-1.000	1.000	-1.000	1.000	1.000
7	-1.000	-1.000	1.000	1.000	-1.000	1.000

```

8 -1.000  1.000 -1.000 -1.000 -1.000 -1.000
9 -1.000 -1.000  1.000  1.000  1.000 -1.000
10 -1.000  1.000 -1.000 -1.000  1.000  1.000
11 -1.000  1.000 -1.000  1.000 -1.000  1.000
12 -1.000 -1.000  1.000 -1.000 -1.000 -1.000
13  1.000  1.000  1.000 -1.000 -1.000  1.000
14  1.000 -1.000 -1.000  1.000 -1.000 -1.000
15  1.000 -1.000 -1.000 -1.000  1.000 -1.000
16  1.000  1.000  1.000  1.000  1.000  1.000

```

Input Response Vector

```

          1
1  0.225
2  0.297
3  0.516
4  0.537
5  0.697
6  0.756
7  0.999
8  0.958
9  0.316
10 0.387
11 0.612
12 0.656
13 0.890
14 0.975
15 1.070
16 1.212

```

```

*****
Significance of Effect Report
*****

```

Label	Half_Effect	Abs_Effect	CL_Upper	Rank	95%Sig
a	0.028227058	0.02822706	0.02898070	12	no
b	0.125963135	0.12596313	0.03833962	14	yes
c	0.250686024	0.25068602	0.04843945	15	yes
d	0.070907904	0.07090790	0.03291497	13	yes
ab	-0.007461889	0.00746189	0.01093157	4	no
ac	0.002247698	0.00224770	0.00592203	1	no
ad	0.014527290	0.01452729	0.02307974	10	no
bc	-0.010901759	0.01090176	0.01642879	7	no
bd	-0.003243873	0.00324387	0.00922863	3	no
cd	0.021311038	0.02131104	0.02580127	11	no

abc	0.002252599	0.00225260	0.00756310	2	no
abd	0.011338698	0.01133870	0.01846654	8	no
acd	0.011558056	0.01155806	0.02066446	9	no
bcd	-0.007494313	0.00749431	0.01268673	5	no
abcd	0.008385358	0.00838536	0.01451179	6	no

Lawson,Grimshaw,and Burt Rn=3.35745 with 1.201 95% Percent.

Corrected Data Report

N	Response	Corr.Resp.	Outlier
1	0.225309282	0.225309282	no
2	0.296665190	0.296665190	no
3	0.515873844	0.515873844	no
4	0.536558443	0.536558443	no
5	0.697229343	0.697229343	no
6	0.755874856	0.755874856	no
7	0.998695158	0.998695158	no
8	0.957607287	0.957607287	no
9	0.315970345	0.315970345	no
10	0.387389826	0.387389826	no
11	0.611723308	0.611723308	no
12	0.656098202	0.656098202	no
13	0.890421019	0.890421019	no
14	0.974511693	0.974511693	no
15	1.070037867	1.176690239	yes
16	1.212187604	1.212187604	no

Perc.	Gap	PSE	Stand.Gap	Critical	Signif.
50th	0.0054916	0.0144653	1.9104971	1.7880000	yes
99th	0.0054916	0.0066234	4.1724537	5.1000000	no

2. Example 2 of submission:

```
print "Example 2 of Submission: nobs=16=2^4, neff=11";
y2 = [ 47.46 49.62 43.13 46.31 51.47 48.49 49.34 46.10
       46.76 48.56 44.83 44.45 59.15 51.33 47.02 47.90 ];
optn = [ 2 ]; /* ipri */
< effrep,outrep,ordat > = urd1out(xdat,y2,optn);
```

Input Response Vector

1
 1 47.46
 2 49.62
 3 43.13
 4 46.31
 5 51.47
 6 48.49
 7 49.34
 8 46.10
 9 46.76
 10 48.56
 11 44.83
 12 44.45
 13 59.15
 14 51.33
 15 47.02
 16 47.90

 Significance of Effect Report

Label	Half_Effect	Abs_Effect	CL_Upper	Rank	95%Sig
a	-0.40000000	0.40000000	0.72215383	5	no
b	-2.11000000	2.11000000	2.40116840	15	no
c	1.85500000	1.85500000	1.92935935	14	no
d	0.50500000	0.50500000	0.89968325	7	no
ab	0.45500000	0.45500000	0.80882073	6	no
ac	-1.24500000	1.24500000	1.67551509	13	no
ad	-0.29000000	0.29000000	0.47792967	2	no
bc	-0.40000000	0.40000000	0.63864843	4	no
bd	-0.59000000	0.59000000	0.99608816	8	no
cd	0.74500000	0.74500000	1.21372274	10	no
abc	0.60000000	0.60000000	1.09987834	9	no
abd	0.36000000	0.36000000	0.55747331	3	no
acd	0.20000000	0.20000000	0.39940279	1	no
bcd	-0.79000000	0.79000000	1.49108302	12	no
abcd	0.76000000	0.76000000	1.34176715	11	no

Lawson, Grimshaw, and Burt Rn=1 with 1.201 95% Percent.

 Corrected Data Report

N	Response	Corr.Resp.	Outlier
1	47.4600000	47.4600000	no
2	49.6200000	49.6200000	no
3	43.1300000	43.1300000	no
4	46.3100000	46.3100000	no
5	51.4700000	51.4700000	no
6	48.4900000	48.4900000	no
7	49.3400000	49.3400000	no
8	46.1000000	46.1000000	no
9	46.7600000	46.7600000	no
10	48.5600000	48.5600000	no
11	44.8300000	44.8300000	no
12	44.4500000	44.4500000	no
13	59.1500000	52.7500000	yes
14	51.3300000	51.3300000	no
15	47.0200000	47.0200000	no
16	47.9000000	47.9000000	no

Perc.	Gap	PSE	Stand.Gap	Critical	Signif.
50th	0.4900000	0.8850000	3.3532267	1.7880000	yes
99th	0.4900000	0.2250000	13.189358	5.1000000	yes

3. Example 3 of submission:

```

print "Defines Linear and Quadratic Orthogonal Main Effects Contrasts";
nobs = 18; neff = 17;
dat1 = [ 1 1 1 1 1 1 1 1 97.94 ,
         1 1 2 2 2 2 2 2 83.40 ,
         1 1 3 3 3 3 3 3 95.88 ,
         1 2 1 1 2 2 3 3 88.86 ,
         1 2 2 2 3 3 1 1 106.58 ,
         1 2 3 3 1 1 2 2 89.57 ,
         1 3 1 2 1 3 2 3 91.98 ,
         1 3 2 3 2 1 3 1 98.41 ,
         1 3 3 1 3 2 1 2 87.56 ,
         2 1 1 3 3 2 2 1 88.11 ,
         2 1 2 1 1 3 3 2 83.81 ,
         2 1 3 2 2 1 1 3 98.27 ,
         2 2 1 2 3 1 3 2 115.52 ,
         2 2 2 3 1 2 1 3 94.89 ,
         2 2 3 1 2 3 2 1 94.70 ,
         2 3 1 3 2 3 1 2 121.62 ,
         2 3 2 1 3 1 2 3 93.86 ,
         2 3 3 2 1 2 3 1 96.10 ];
cnam = [" A G B C D E F H Y "];

```

```

dat1 = cname(dat1,cnam);
yvec = dat1[,9]; print "Dat1=",dat1;

effnam = [" A1 G1 Gq B1 Bq C1 Cq D1 Dq E1
          Eq F1 Fq H1 Hq ALG1 ALGq "];
dat2 = cons(nobs,neff,.);
print "This will make the X'X matrix diagonal";
for (i = 1; i <= nobs; i++) {
  dat2[i, 1] = 2*dat1[i,1] - 3;          /* A1 */
  dat2[i, 2] = dat1[i,2] - 2;          /* G1 */
  dat2[i, 3] = (dat1[i,2] == 2) ? -2 : 1; /* Gq */
  dat2[i, 4] = dat1[i,3] - 2;          /* B1 */
  dat2[i, 5] = (dat1[i,3] == 2) ? -2 : 1; /* Bq */
  dat2[i, 6] = dat1[i,4] - 2;          /* C1 */
  dat2[i, 7] = (dat1[i,4] == 2) ? -2 : 1; /* Cq */
  dat2[i, 8] = dat1[i,5] - 2;          /* D1 */
  dat2[i, 9] = (dat1[i,5] == 2) ? -2 : 1; /* Dq */
  dat2[i,10] = dat1[i,6] - 2;          /* E1 */
  dat2[i,11] = (dat1[i,6] == 2) ? -2 : 1; /* Eq */
  dat2[i,12] = dat1[i,7] - 2;          /* F1 */
  dat2[i,13] = (dat1[i,7] == 2) ? -2 : 1; /* Fq */
  dat2[i,14] = dat1[i,8] - 2;          /* H1 */
  dat2[i,15] = (dat1[i,8] == 2) ? -2 : 1; /* Hq */
  /* Defines Interactions to Make X1 Full Rank; */
  dat2[i,16] = dat2[i,1] * dat2[i,2]; /* ALGL=AL*GL; */
  dat2[i,17] = dat2[i,1] * dat2[i,3]; /* ALGQ=AL*GQ; */
}
print "Dat2=", dat2;

ps = "X'X matrix will be equal";
print "Standardize Contrasts so that diagonals of", ps;
fac1 = 1. / sqrt(2. * 9.);
fac2 = 1. / sqrt(2. * 6.);
fac3 = 1. / sqrt(6. * 6.);
xdat = cons(nobs,neff,.);
xdat[,1] = fac1 * dat2[,1];
for (i = 2; i < 17; i+=2) {
  xdat[,i ] = fac2 * dat2[,i ];
  xdat[,i+1] = fac3 * dat2[,i+1];
}
xdat = cname(xdat,effnam);
print "Standardized Xdat=",xdat;

optn = [ 2 ]; /* ipri */

```



```
< effrep,outrep,cordat > = urdlout(xdat,yvec,optn);
```

```
*****
Analysis of Unreplicated 2^k and 2^(k-p) Designs (Lawson, 2007)
*****
```

```
Number of Observations . . . . . 18
Number of Effects. . . . . 17
```

Input Design Matrix

	A1	G1	Gq	B1	Bq	C1	Cq	D1	Dq
1	-0.236	-0.289	0.167	-0.289	0.167	-0.289	0.167	-0.289	0.167
2	-0.236	-0.289	0.167	0.000	-0.333	0.000	-0.333	0.000	-0.333
3	-0.236	-0.289	0.167	0.289	0.167	0.289	0.167	0.289	0.167
4	-0.236	0.000	-0.333	-0.289	0.167	-0.289	0.167	0.000	-0.333
5	-0.236	0.000	-0.333	0.000	-0.333	0.000	-0.333	0.289	0.167
6	-0.236	0.000	-0.333	0.289	0.167	0.289	0.167	-0.289	0.167
7	-0.236	0.289	0.167	-0.289	0.167	0.000	-0.333	-0.289	0.167
8	-0.236	0.289	0.167	0.000	-0.333	0.289	0.167	0.000	-0.333
9	-0.236	0.289	0.167	0.289	0.167	-0.289	0.167	0.289	0.167
10	0.236	-0.289	0.167	-0.289	0.167	0.289	0.167	0.289	0.167
11	0.236	-0.289	0.167	0.000	-0.333	-0.289	0.167	-0.289	0.167
12	0.236	-0.289	0.167	0.289	0.167	0.000	-0.333	0.000	-0.333
13	0.236	0.000	-0.333	-0.289	0.167	0.000	-0.333	0.289	0.167
14	0.236	0.000	-0.333	0.000	-0.333	0.289	0.167	-0.289	0.167
15	0.236	0.000	-0.333	0.289	0.167	-0.289	0.167	0.000	-0.333
16	0.236	0.289	0.167	-0.289	0.167	0.289	0.167	0.000	-0.333
17	0.236	0.289	0.167	0.000	-0.333	-0.289	0.167	0.289	0.167
18	0.236	0.289	0.167	0.289	0.167	0.000	-0.333	-0.289	0.167

Input Design Matrix

	E1	Eq	F1	Fq	H1	Hq	AlG1	AlGq
1	-0.289	0.167	-0.289	0.167	-0.289	0.167	0.289	-0.167
2	0.000	-0.333	0.000	-0.333	0.000	-0.333	0.289	-0.167
3	0.289	0.167	0.289	0.167	0.289	0.167	0.289	-0.167
4	0.000	-0.333	0.289	0.167	0.289	0.167	0.000	0.333
5	0.289	0.167	-0.289	0.167	-0.289	0.167	0.000	0.333
6	-0.289	0.167	0.000	-0.333	0.000	-0.333	0.000	0.333
7	0.289	0.167	0.000	-0.333	0.289	0.167	-0.289	-0.167
8	-0.289	0.167	0.289	0.167	-0.289	0.167	-0.289	-0.167
9	0.000	-0.333	-0.289	0.167	0.000	-0.333	-0.289	-0.167
10	0.000	-0.333	0.000	-0.333	-0.289	0.167	-0.289	0.167

11	0.289	0.167	0.289	0.167	0.000	-0.333	-0.289	0.167
12	-0.289	0.167	-0.289	0.167	0.289	0.167	-0.289	0.167
13	-0.289	0.167	0.289	0.167	0.000	-0.333	0.000	-0.333
14	0.000	-0.333	-0.289	0.167	0.289	0.167	0.000	-0.333
15	0.289	0.167	0.000	-0.333	-0.289	0.167	0.000	-0.333
16	0.289	0.167	-0.289	0.167	0.000	-0.333	0.289	0.167
17	-0.289	0.167	0.000	-0.333	0.289	0.167	0.289	0.167
18	0.000	-0.333	0.289	0.167	-0.289	0.167	0.289	0.167

Input Response Vector

	1
1	97.94
2	83.40
3	95.88
4	88.86
5	106.6
6	89.57
7	91.98
8	98.41
9	87.56
10	88.11
11	83.81
12	98.27
13	115.5
14	94.89
15	94.70
16	121.6
17	93.86
18	96.10

Significance of Effect Report

Label	Half_Effect	Abs_Effect	CL_Upper	Rank	95%Sig
A1	11.00729556	11.0072956	13.0848080	11	no
G1	12.15899667	12.1589967	19.0494817	15	no
Gq	-7.216666667	7.21666667	8.41923908	6	no
B1	-12.10992190	12.1099219	17.1266856	14	no
Bq	7.368333333	7.36833333	9.25291187	7	no
C1	12.05218687	12.0521869	15.5773027	13	no
Cq	-8.081666667	8.08166667	10.1239829	8	no
D1	9.589787971	9.58978797	12.0234517	10	no
Dq	-4.786666667	4.78666667	6.83284397	4	no

E1	0.288675135	0.28867513	4.56943981	1	no
Eq	18.38333333	18.3833333	26.6818495	17	no
F1	-8.163732806	8.16373281	11.0428885	9	no
Fq	17.03333333	17.0333333	21.7090453	16	no
H1	-5.225019936	5.22501994	7.61477213	5	no
Hq	-2.896666667	2.89666667	6.06783619	3	no
AlG1	11.73753097	11.7375310	14.2548883	12	no
AlGq	-2.266666667	2.26666667	5.31484600	2	no

Lawson,Grimshaw,and Burt Rn=1 with 1.178 95% Percent.

Corrected Data Report

N	Response	Corr.Resp.	Outlier
1	97.94000000	97.94000000	no
2	83.40000000	83.40000000	no
3	95.88000000	95.88000000	no
4	88.86000000	88.86000000	no
5	106.5800000	106.5800000	no
6	89.57000000	89.57000000	no
7	91.98000000	91.98000000	no
8	98.41000000	98.41000000	no
9	87.56000000	87.56000000	no
10	88.11000000	88.11000000	no
11	83.81000000	83.81000000	no
12	98.27000000	98.27000000	no
13	115.5200000	115.5200000	no
14	94.89000000	94.89000000	no
15	94.70000000	94.70000000	no
16	121.6200000	29.03181091	yes
17	93.86000000	93.86000000	no
18	96.10000000	96.10000000	no

Perc.	Gap	PSE	Stand.Gap	Critical	Signif.
50th	2.5553418	12.245599	1.4309717	1.7880000	no
99th	2.5553418	22.013582	0.7960134	5.1000000	no