```
*************************************************************************;
** This Program finds optimal design using exchange algorithm under the     ***;
** psi-J criterion that integrates over the prior distributions of          ***;
** Lambda where Lambda is of form aI+bJ or a more general form.             ***;
** Monte Carlo method is used.                                              ***;
*************************************************************************;

options  ls=max ps=max nocenter notes;
libname mylib 'U:\data';


proc iml;

%** set initial seed for the random generation of the initial design matrix **;
nseed=614292;
*nseed=1025;
*nseed=10082005;
*nseed=6718;

%** initial value for the call ranuni statement, not used in later program  **;
rrr=0;

%** initial seed for genetation of Lambdas and sigmasqure **;
seed=886;

%** number of repeated searches with different initial designs **;
nint=10;

%** number of iterations in the Monte Carlo procedure to evaluate the integral**;
%** over Lambda and sigmasquare                                              **;
nlam=10000;


%** Input the number of levels for each factor. For example, if there are **;
%** 5 factors with (2,3,4,2,3) levels, define factors={2,3,4,2,3}.        **;
%** The # of levels can only be 2, 3, or 4.                               **;
*factors={2,2};
factors={2,2,2};

%** Number of trials                                                      **;
*n_trials=12;
n_trials=16;

%** Are there initial designs (1=yes 0=no)?                               **;
has_init=0;
```

```
%** Initial design (needed if has_init=1)                                  **;
*init=;

%** Specify number of initial trials to be generated randomly              **;
n_init = 4;

%** Specify d/a ratio in Lambda0                                 **;
a=1;
*b=0;
*b=0.5;
*b=1;
*b=2;
*b=10;
*b=-0.1;
b=-0.25;

%** number of parameters (not including the intercept)     **;
p=sum(factors) - nrow(factors) + 1;
JM=j(p,p,1);
print p;

%** prior parameters for Lambda**;
eta0=p+2;
Lambda0=a*i(p) + b*JM;

**Lambda0={
0.4731985 0.1895264 0.4647651,
0.1895264 5.4975212 0.241813,
0.4647651 0.241813  0.4772845};

**Lambda0={
  1.42808 0.1554487 2.6176585,
0.1554487 0.1017228 0.3051262,
2.6176585 0.3051262 5.0187351};

sigmas=1;

%** Specify max number of iterations                                      **;
max_iteration = 10000;

%************************************************************;
%* coefficients of standardized orthogonal contrasts         **;
%* for factors with 2,3 and 4 levels. This program is        **;
%* limited to factors that contain less than 4 levels        **;
%* it can be modified to accommodate factors with more levels**;
```

```
%*************************************************************;

d2={-1,
     1};

d3={-1.22 -0.71,
     0     1.41,
     1.22 -0.71};

d4={-1.41 -0.82 -0.58,
     0     1.63 -0.58,
     0     0     1.73,
     1.41 -0.82 -0.58};

*************************************************************;
*** this function generates a random draw from multi-variate    ***;

*** normal(u,v), where u is mean vector, v is covariance matrix ***;
*************************************************************;
start multnorm(u,v,seed);

if (ncol(v)^=nrow(v)) | (nrow(u)^=nrow(v)) then do;
  print "ERROR!!";
  stop;
end;

n=nrow(u);
x=j(n,1,0);
xtemp=0;
do i=1 to n;
  call rannor(seed,xtemp);
  x[i]=xtemp;
end;

y=(root(v))`*x + u;
return(y);

finish multnorm;

************************************************************************;
*** this function generates a random draw from inverted wishart distr **;
*** et is the prior degree of freedom, dt is the variance matrix      **;
************************************************************************;
start iw(et,dt,seed);

u=j(nrow(dt),1,0);
```

```
do i=1 to et;
  w=multnorm(u,dt,seed + i*123456789);
  if i=1 then z=w;
  else z=z||w;
end;

return(inv(z*z`));

finish iw;

%*************************************************************;
%* Create all candidate design points x                     **;
%*************************************************************;

num_factors = nrow(factors);

if num_factors > 10 then do;
  print "ERROR: NUMBER OF FACTORS EXCEEDS 10 !!!";
  stop;
end;

factors_exp = factors;
do i=1 to 10-num_factors;
  factors_exp = factors_exp // {1};
end;

levels=j(10,1,0);

do i=1 to 10;
  levels[i] = factors_exp[i,1];
end;

if levels[1]=2 then m1=d2;
  else if levels[1]=3 then m1=d3;
  else if levels[1]=4 then m1=d4;
if levels[2]=2 then m2=d2;
  else if levels[2]=3 then m2=d3;
  else if levels[2]=4 then m2=d4;
if levels[3]=2 then m3=d2;
  else if levels[3]=3 then m3=d3;
  else if levels[3]=4 then m3=d4;
if levels[4]=2 then m4=d2;
  else if levels[4]=3 then m4=d3;
  else if levels[4]=4 then m4=d4;
if levels[5]=2 then m5=d2;
```

```
  else if levels[5]=3 then m5=d3;
  else if levels[5]=4 then m5=d4;
if levels[6]=2 then m6=d2;
  else if levels[6]=3 then m6=d3;
  else if levels[6]=4 then m6=d4;
if levels[7]=2 then m7=d2;
  else if levels[7]=3 then m7=d3;
  else if levels[7]=4 then m7=d4;
if levels[8]=2 then m8=d2;
  else if levels[8]=3 then m8=d3;
  else if levels[8]=4 then m8=d4;
if levels[9]=2 then m9=d2;
  else if levels[9]=3 then m9=d3;
  else if levels[9]=4 then m9=d4;
if levels[10]=2 then m10=d2;
  else if levels[10]=3 then m10=d3;
  else if levels[10]=4 then m10=d4;


%** number of candidate designs                              **;
cand_n = 1;
do i=1 to nrow(factors);
  cand_n=cand_n*factors[i];
end;

do i1 = 1 to levels[1];
do i2 = 1 to levels[2];
do i3 = 1 to levels[3];
do i4 = 1 to levels[4];
do i5 = 1 to levels[5];
do i6 = 1 to levels[6];
do i7 = 1 to levels[7];
do i8 = 1 to levels[8];
do i9 = 1 to levels[9];
do i10 = 1 to levels[10];
  x=m1[i1,];  d=i1;
  if levels[2]>1 then do;  x=x||m2[i2,]; d=d||i2;  end;
  if levels[3]>1 then do;  x=x||m3[i3,]; d=d||i3;  end;
  if levels[4]>1 then do;  x=x||m4[i4,]; d=d||i4;  end;
  if levels[5]>1 then do;  x=x||m5[i5,]; d=d||i5;  end;
  if levels[6]>1 then do;  x=x||m6[i6,]; d=d||i6;  end;
  if levels[7]>1 then do;  d=x||m7[i7,]; d=d||i7;  end;
  if levels[8]>1 then do;  d=x||m8[i8,]; d=d||i8;  end;
  if levels[9]>1 then do;  d=x||m9[i9,]; d=d||i9;  end;
  if levels[10]>1 then do; d=x||m10[i10,]; d=d||i10; end;
```

```
  if i1=1 & i2=1 & i3=1 & i4=1 & i5=1 &
     i6=1 & i7=1 & i8=1 & i9=1 & i10=1 then do;
       cand_x=x;
           cand_d=d;
  end;
  else do;
       cand_x=cand_x//x;
       cand_d=cand_d//d;
  end;
end;
end;
end;
end;
end;
end;
end;
end;
end;
end;

cand_x= j(nrow(cand_x),1,1) || cand_x;

%** print cand_x, cand_d;

if nrow(cand_x) ^= cand_n then do;
  print "Error: number of candidate designs is incorrect!!";
  stop;
end;
if ncol(cand_x) ^= p then do;
  print "Error: number of parameters is incorrect!!";
  stop;
end;


%*************************************************************;
%* create initial design matrix                              **;
%*************************************************************;

mydet=j(1,nint,0);

do myr=1 to nint;
        call ranuni(nseed,rrr);

        if has_init=1 then do;
          init_d=init;
          init_n=nrow(init);
```

```
  do i=1 to nrow(init_d);
    x={1};
        do j=1 to ncol(init_d);
          k=init_d[i,j];
      if factors[j]=2 then x=x||d2[k,];
          if factors[j]=3 then x=x||d3[k,];
          if factors[j]=4 then x=x||d4[k,];
        end;
        if i=1 then init_x=x;
        else init_x=init_x//x;
  end;
 end;

 iflag=0;
 if has_init=0 then do;
  do while (iflag<1);
   init_n = n_init;

   do i=1 to init_n;
     ran=ranuni(nseed);
     index=ceil(ran*cand_n);

         if i=1 then do;
       init_x=cand_x[index,];
          init_d=cand_d[index,];
        end;
        else do;
          init_x=init_x//cand_x[index,];
          init_d=init_d//cand_d[index,];
        end;
   end;
   xpx_init=init_x`*init_x;
   eig_init=eigval(xpx_init);
   if min(eig_init)>0 & det(xpx_init)>0 then iflag=1;

  end;
 end;

 if init_n > n_trials then do;
   print "Error: number of initial designs exceeds the number of trials!!!";
   stop;
end;


%*****************************************************************;
```

```
%* sequentially add to n_trials                                          **;
%*************************************************************************;

design_x = init_x;
design_d = init_d;
pp=p*(p+1)/2;
flam=j(pp,pp,0);
rr=j(1,pp,0);
cc=j(1,pp,0);
do i=1 to p;
do j=i to p;
    t=(i-1)*p+j-i*(i-1)/2;
cc[t]=j;
rr[t]=i;
end;
end;

do i=1 to n_trials - init_n ;

  do j=1 to cand_n;
    x=cand_x[j,];
        det_all=j(1,nlam,0);
        do lam=1 to nlam;

           Lambda=iw(eta0,inv(Lambda0),lam+seed);

           den_temp1 = design_x'*design_x + x'*x;
           den_temp2 = sigmas*i(p)+ Lambda*design_x'*design_x + Lambda*x'*x;
           ftheta=den_temp1*inv(den_temp2);

           do mk=1 to pp;
             do mc=mk to pp;
                if (rr[mk]=cc[mk] & rr[mc]=cc[mc]) then
                   flam[mk,mc]=(ftheta[rr[mk],cc[mc]]**2)/2;
                else if (rr[mk]=cc[mk] | rr[mc]=cc[mc]) then
                   flam[mk,mc]=ftheta[rr[mk],rr[mc]]*ftheta[cc[mk],cc[mc]];
                else flam[mk,mc]=ftheta[rr[mk],rr[mc]]*ftheta[cc[mk],cc[mc]]+
                                 ftheta[cc[mk],rr[mc]]*ftheta[rr[mk],cc[mc]];
                flam[mc,mk]=flam[mk,mc];
             end;
           end;

           det_all[lam]=log((det(den_temp1)/det(den_temp2))*det(flam));
        end;

        det_add=sum(det_all)/ncol(det_all);
```

```
    if j=1 then do;
      max_det_add=det_add;
          max_index = 1;
        end;
        else do;
          if det_add > max_det_add then do;
            max_det_add = det_add;
                max_index = j ;
          end;
        end;
  end;

  x= cand_x[max_index,];
  d= cand_d[max_index,];
  design_x = design_x // x ;
  design_d = design_d // d;
  max_det=max_det_add;
end;

%************************************************************;
%** apply exchange algorithm                                **;
%************************************************************;

flag=0;
do i=1 to max_iteration until(flag);

  %****************************************;
  %*  add one design point                **;
  %****************************************;

  do j=1 to cand_n;
    x=cand_x[j,];
        det_all=j(1,nlam,0);
        do lam=1 to nlam;

           Lambda=iw(eta0,inv(Lambda0),lam+seed);
           den_temp1 = design_x'*design_x + x'*x;
           den_temp2 = sigmas*i(p)+ Lambda*design_x'*design_x + Lambda*x'*x;
           ftheta=den_temp1*inv(den_temp2);

           do mk=1 to pp;
             do mc=mk to pp;
                if (rr[mk]=cc[mk] & rr[mc]=cc[mc]) then
                   flam[mk,mc]=(ftheta[rr[mk],cc[mc]]**2)/2;
                else if (rr[mk]=cc[mk] | rr[mc]=cc[mc]) then
```

```
                flam[mk,mc]=ftheta[rr[mk],rr[mc]]*ftheta[cc[mk],cc[mc]];
              else flam[mk,mc]=ftheta[rr[mk],rr[mc]]*ftheta[cc[mk],cc[mc]]+
                                ftheta[cc[mk],rr[mc]]*ftheta[rr[mk],cc[mc]];
              flam[mc,mk]=flam[mk,mc];
            end;
          end;
          det_all[lam]=log((det(den_temp1)/det(den_temp2))*det(flam));
       end;

       det_add=sum(det_all)/ncol(det_all);

  if j=1 then do;
    max_det_add=det_add;
        max_index = 1;
       end;
       else do;
         if det_add > max_det_add then do;
           max_det_add = det_add;
               max_index = j ;
         end;
       end;
end;

max_index_add = max_index;

x_add = cand_x[max_index,];
d_add = cand_d[max_index,];
design_x1 = design_x // x_add ;
design_d1 = design_d // d_add;

%***********************************;
%** delete one design point        **;
%***********************************;

design_x1_n = nrow(design_x1);

do j=1 to design_x1_n;
  x=design_x1[j,];
       det_all=j(1,nlam,0);
       do lam=1 to nlam;

          Lambda=iw(eta0,inv(Lambda0),lam+seed);

          den_temp3 = design_x'*design_x - x'*x;
          den_temp4 = sigmas*i(p)+ Lambda*den_temp3;
          ftheta=den_temp3*inv(den_temp4);
```

```
         do mk=1 to pp;
           do mc=mk to pp;
              if (rr[mk]=cc[mk] & rr[mc]=cc[mc]) then
                 flam[mk,mc]=(ftheta[rr[mk],cc[mc]]**2)/2;
              else if (rr[mk]=cc[mk] | rr[mc]=cc[mc]) then
                 flam[mk,mc]=ftheta[rr[mk],rr[mc]]*ftheta[cc[mk],cc[mc]];
              else flam[mk,mc]=ftheta[rr[mk],rr[mc]]*ftheta[cc[mk],cc[mc]]+
                                  ftheta[cc[mk],rr[mc]]*ftheta[rr[mk],cc[mc]];
              flam[mc,mk]=flam[mk,mc];
           end;
         end;

         det_all[lam]=log((det(den_temp3)/det(den_temp4))*det(flam));
       end;

       det_del=sum(det_all)/ncol(det_all);

  if j=1 then do;
    max_det_del=det_del;
        max_index = 1;
       end;
       else do;
         if det_del > max_det_del then do;
           max_det_del = det_del;
               max_index = j ;
         end;
       end;
end;

max_index_del = max_index;

x_del= design_x1[max_index,];
d_del= design_d1[max_index,];

       if max_index_del=1 then do;
                 design_x2=design_x1[2:design_x1_n,];
                 design_d2=design_d1[2:design_x1_n,];

       end;
       else do;
                 design_x2=design_x1[1:(max_index_del-1),]
                             //design_x1[(max_index_del+1):design_x1_n,];
                 design_d2=design_d1[1:(max_index_del-1),]
                            //design_d1[(max_index_del+1):design_x1_n,];
       end;
```

```
  max_det2=max_det_del;

  if max_det2 > max_det then do;
    max_det=max_det2;
        design_x=design_x2;
        design_d=design_d2;
  end;
  else do;
    flag=1;
    print "Exchange does not improve criterion.";
    print "Final design:";
        print design_x, design_d ;
        print "Criterion Max:";
        print max_det;
        print "xpx";
        xpx=design_x'*design_x;
        print xpx;
  end;
end;

if i=max_iteration+1 then do;
  print "Maximum number of iterations is reached";
  print "Final design:";
  print design_x, design_d;
  print "Criterion Max:";
  print max_det;
  xpx=design_x'*design_x;
  print "xpx";
  print xpx;
end;

mydet[myr]=max_det;

end;

print mydet;

mymax=max(mydet);
print mymax;
```