Serie 11: Mixture designs

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Problem 1

Question a

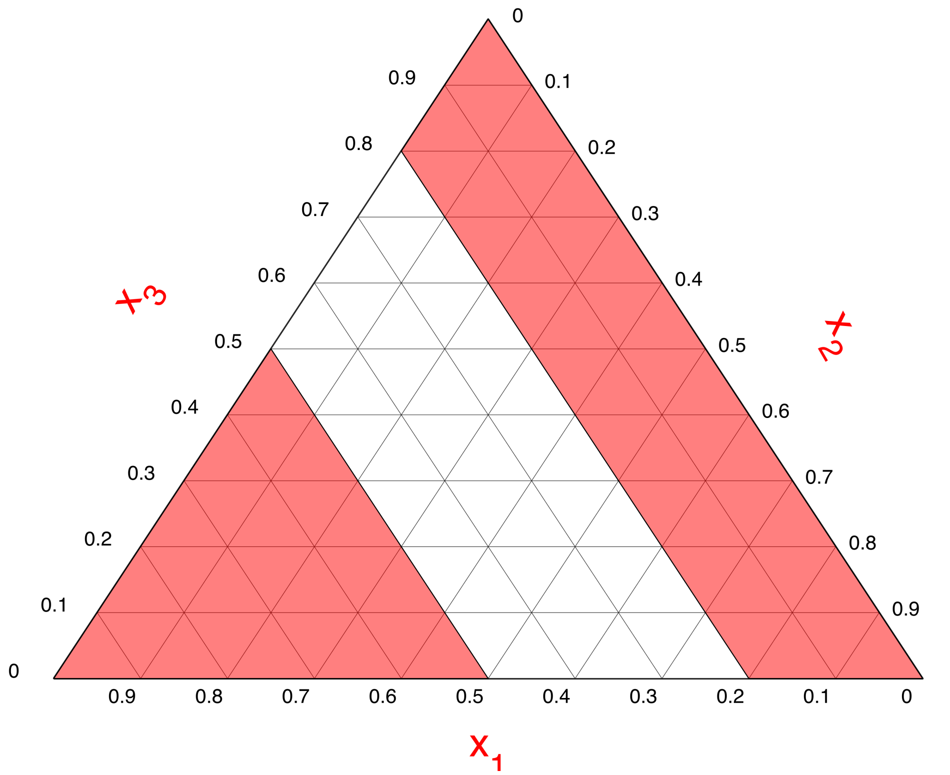
On a ternary diagram whose variables are x_1, x_2 and x_3, determine the domains corresponding to the following constraints:

$20\% \leq x_1 \leq 50\%$

- The possible area is colored in white and the prohibited area is colored in red
- It's much faster to do this by hand!
- The axis scales are reversed compared to what was shown in the course due to the use of the ternaxes() routine

```
% Preparing the ternary axes
ternaxes;
h1=ternlabel('x_1','x_2','x_3');
set(h1(1),'FontSize',20,'Color','r','Position',[.5, -.1, 0])
set(h1(2),'FontSize',20,'Color','r','Position',[.9, .45, 0])
set(h1(3),'FontSize',20,'Color','r','Position',[.10, .5, 0])

% Indicating the zones
```

```
hold on
[w1,w2]=terncoords([.2 .2 0  0],[0 .8 1 0]); % x1 > 0.0
patch(w1,w2,[1 0 0],'FaceAlpha',.5);
[w1,w2]=terncoords([.5 .5 1],[0 .5 0]); % x1 < 0.5
patch(w1,w2,[1 0 0],'FaceAlpha',.5);
hold off
```



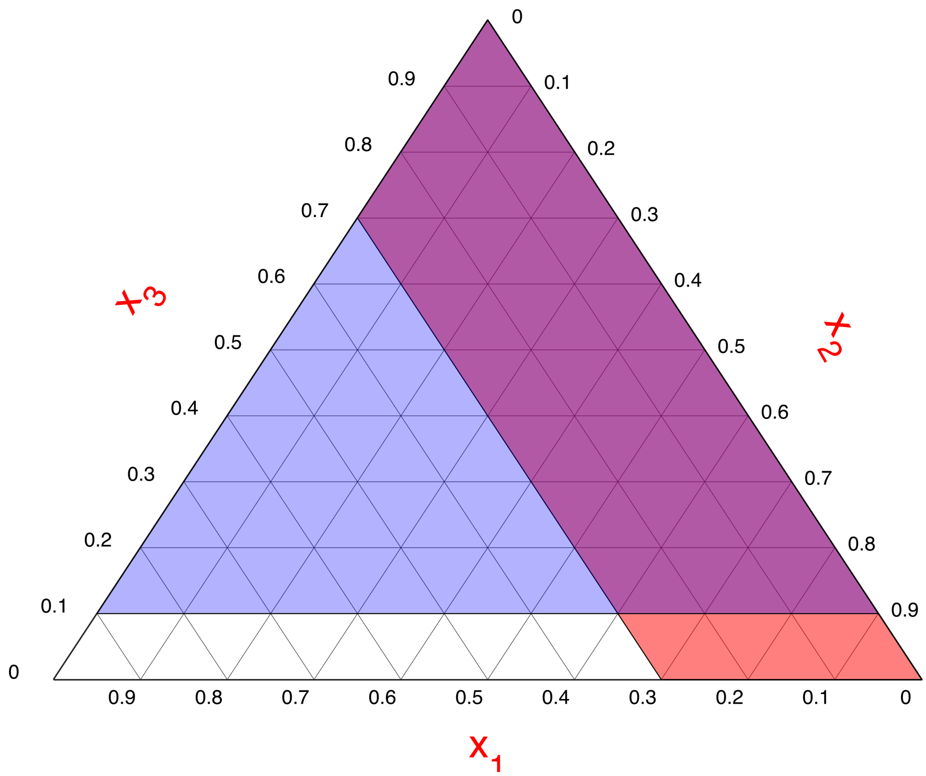
Question b

On a ternary diagram whose variables are x_1, x_2 and x_3, determine the domains corresponding to the following constraints:

$$\begin{cases} x_1 \geq 30\% \\ x_3 \leq 10\% \end{cases}$$

```
% Preparing the ternary axes
ternaxes;
h1=ternlabel('x_1','x_2','x_3');
set(h1(1),'FontSize',20,'Color','r','Position',[.5, -.1, 0])
set(h1(2),'FontSize',20,'Color','r','Position',[.9, .45, 0])
set(h1(3),'FontSize',20,'Color','r','Position',[.10, .5, 0])

% Indicating the zones
hold on
```

```
[w1,w2]=terncoords([.3 .3 0 0],[0 .7 1 0]); % x1 > 0.3
patch(w1,w2,[1 0 0],'FaceAlpha',.5);
[w1,w2]=terncoords([.9 0 0],[0 .9 0]); % x3 < 0.1
patch(w1,w2,[0 0 1],'FaceAlpha',.3);
hold off
```



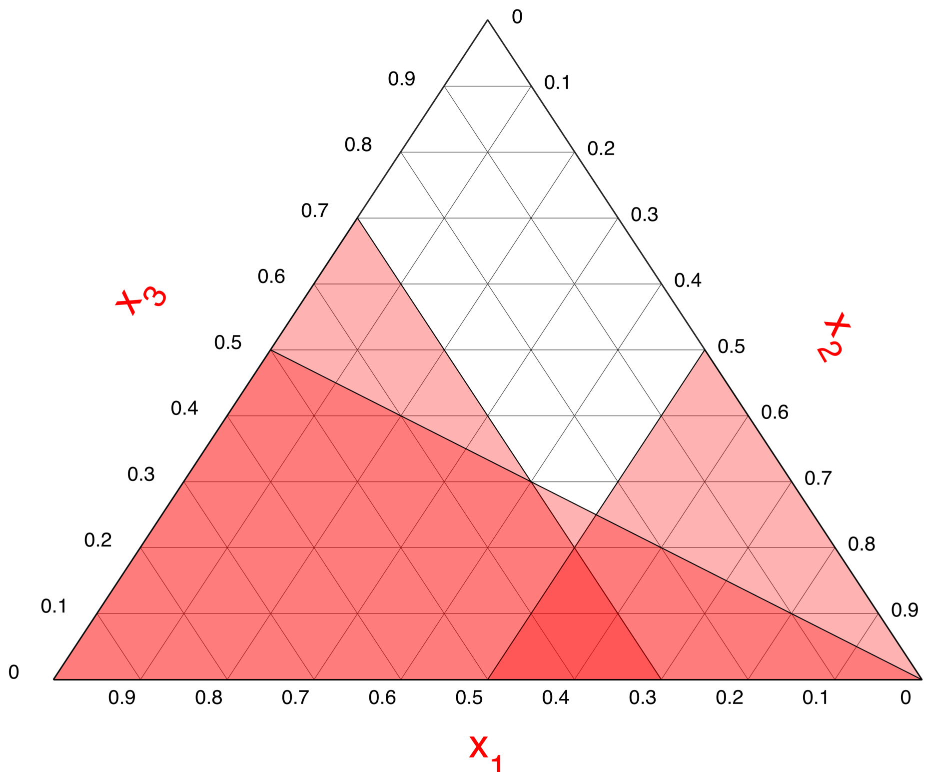
Question c

On a ternary diagram whose variables are x_1, x_2 and x_3, determine the domains corresponding to the following constraints:

$$\begin{cases} x_1 \leq 30\% \\ x_2 \leq 50\% \\ x_1 \leq x_3 \end{cases}$$

```
% Preparing the ternary axes
ternaxes;
h1=ternlabel('x_1','x_2','x_3');
set(h1(1),'FontSize',20,'Color','r','Position',[.5, -.1, 0])
set(h1(2),'FontSize',20,'Color','r','Position',[.9, .45, 0])
set(h1(3),'FontSize',20,'Color','r','Position',[.10, .5, 0])

% Indicating the zones
hold on
[w1,w2]=terncoords([.3 .3 1 ],[0 .7 0 ]); % x1 < 0.3
patch(w1,w2,[1 0 0],'FaceAlpha',.3);
```

```
[w1,w2]=terncoords([0 0 .5],[1 .5 .5]); % x2 < 0.5
patch(w1,w2,[1 0 0],'FaceAlpha',.3);
[w1,w2]=terncoords([0 1 .5 ],[1 0 0 ]); % x1 < x3
patch(w1,w2,[1 0 0],'FaceAlpha',.3);
hold off
```



Question d

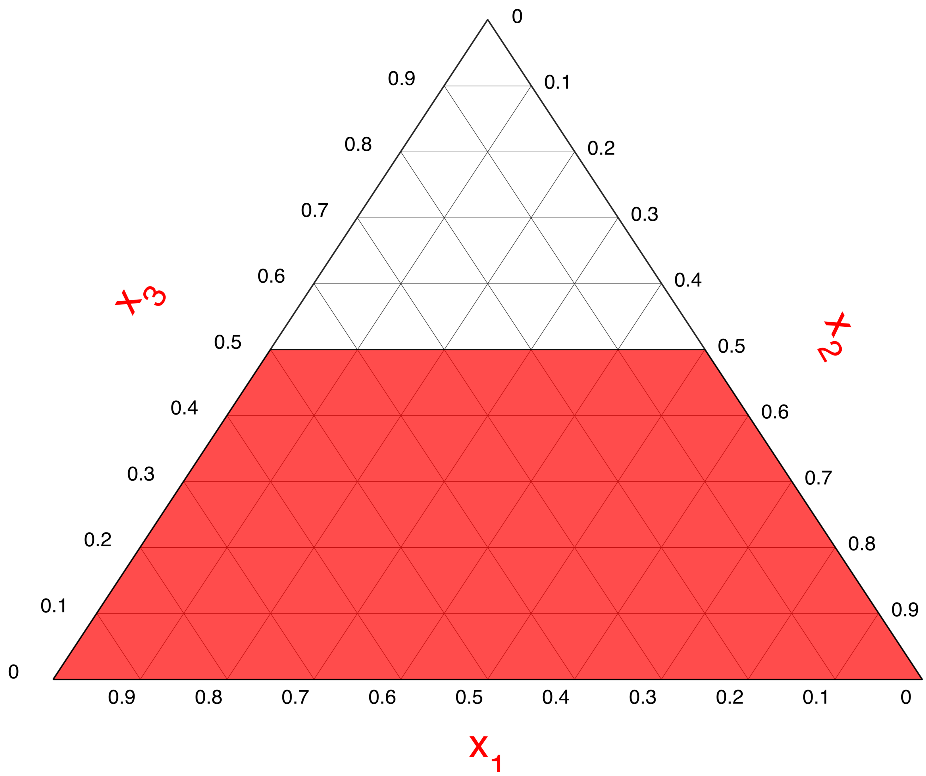
On a ternary diagram whose variables are x_1, x_2 and x_3, determine the domains corresponding to the following constraints:

$x_1 + x_2 \leq x_3$

This experssion is equivalent to $1 - x_3 \leq x_3$ therefore $\frac{1}{2} \leq x_3$

```
% Preparing the ternary axes
ternaxes;
h1=ternlabel('x_1','x_2','x_3');
set(h1(1),'FontSize',20,'Color','r','Position',[.5, -.1, 0])
set(h1(2),'FontSize',20,'Color','r','Position',[.9, .45, 0])
set(h1(3),'FontSize',20,'Color','r','Position',[.10, .5, 0])
```

```
% Indicating the zones
hold on
[w1,w2]=terncoords([0 .5  1 0],[.5 0 0 1]); % x1 < 0.3
patch(w1,w2,[1 0 0],'FaceAlpha',.7);
hold off
```



Problem 2

1. Built a $\{3,3\}$ simplex lattice design
2. Placing measurement points on a ternary diagram
3. Built a $\{4,3\}$ simplex lattice design
4. Draw an axonométry of the design

Compute the coordinates $\{3,3\}$ simplex lattice design

```
% 3 variables de 3 niveaux
S3=(fullfact([4 4 4])-1)/3;
index=sum(S3,2)==1;
S3=S3(index,:);
```

To obtain a fraction format, one can transform the matrix of experiments into a symbolic object:

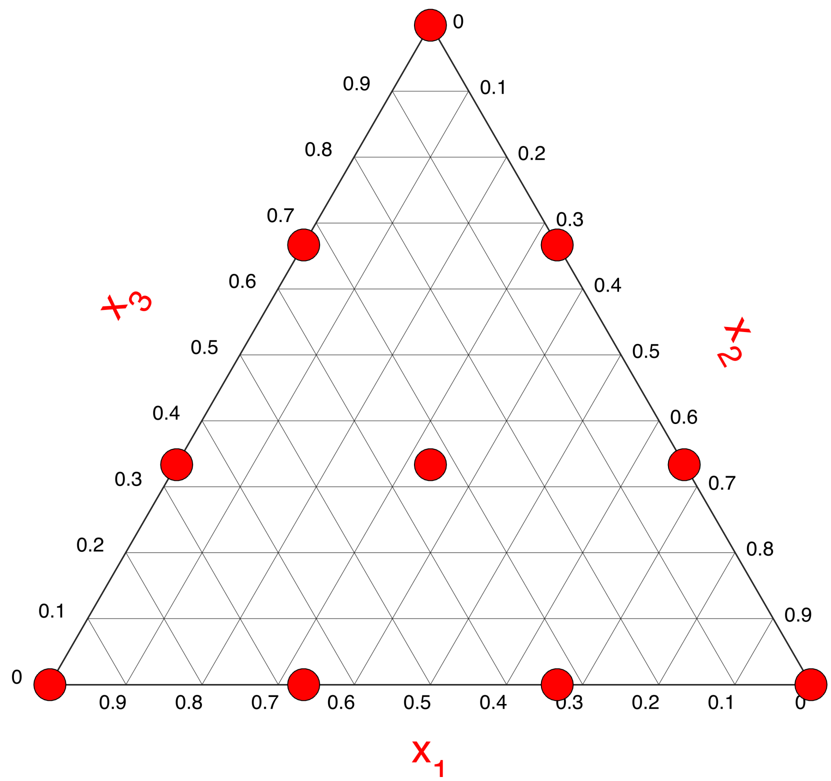
```
SS=sym(S3)
```

```
SS =
```

$$\begin{pmatrix} 1 & 0 & 0 \\ \frac{2}{3} & \frac{1}{3} & 0 \\ \frac{1}{3} & \frac{2}{3} & 0 \\ 0 & 1 & 0 \\ \frac{2}{3} & 0 & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ 0 & \frac{2}{3} & \frac{1}{3} \\ \frac{1}{3} & 0 & \frac{2}{3} \\ 0 & \frac{1}{3} & \frac{2}{3} \\ 0 & 0 & 1 \end{pmatrix}$$

Placing the data point on the ternary diagram

```
h=ternplot(S3(:,1),S3(:,2),S3(:,3),'ok');
set(h,'MarkerSize',16,'MarkerFaceColor','r')
h1=ternlabel('x_1','x_2','x_3');
set(h1(1),'FontSize',20,'Color','r','Position',[.5, -.1, 0])
set(h1(2),'FontSize',20,'Color','r','Position',[.9, .45, 0])
set(h1(3),'FontSize',20,'Color','r','Position',[.10, .5, 0])
```



Compute the coordinates $\{4, 3\}$ simplex lattice design

```
% 4 variables with 4 levels
S4=(fullfact([4 4 4 4])-1)/3;
index=sum(S4,2)==1;
S4=S4(index,:);
```

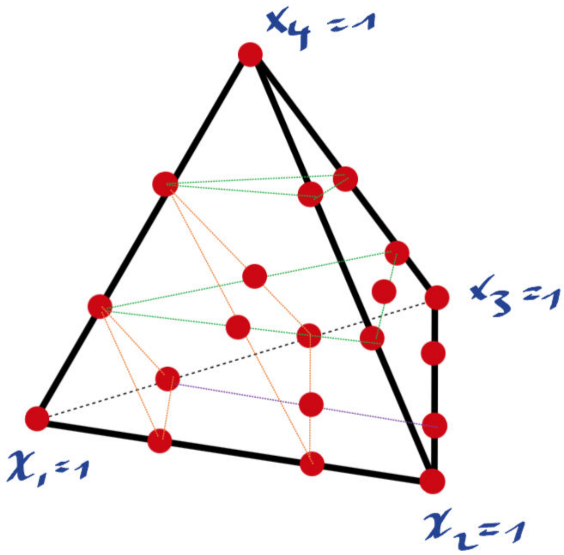
To obtain a fraction format, one can transform the matrix of experiments into a symbolic object:

```
SS=sym(S4)
```

```
SS =
```

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ \frac{2}{3} & \frac{1}{3} & 0 & 0 \\ \frac{1}{3} & \frac{2}{3} & 0 & 0 \\ 0 & 1 & 0 & 0 \\ \frac{2}{3} & 0 & \frac{1}{3} & 0 \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} & 0 \\ 0 & \frac{2}{3} & \frac{1}{3} & 0 \\ \frac{1}{3} & 0 & \frac{2}{3} & 0 \\ 0 & \frac{1}{3} & \frac{2}{3} & 0 \\ 0 & 0 & 1 & 0 \\ \frac{2}{3} & 0 & 0 & \frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & 0 & \frac{1}{3} \\ 0 & \frac{2}{3} & 0 & \frac{1}{3} \\ \frac{1}{3} & 0 & \frac{1}{3} & \frac{1}{3} \\ 0 & \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ 0 & 0 & \frac{2}{3} & \frac{1}{3} \\ \frac{1}{3} & 0 & 0 & \frac{2}{3} \\ 0 & \frac{1}{3} & 0 & \frac{2}{3} \\ 0 & 0 & \frac{1}{3} & \frac{2}{3} \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

3D representation



Problem 3

Matrix of experiments

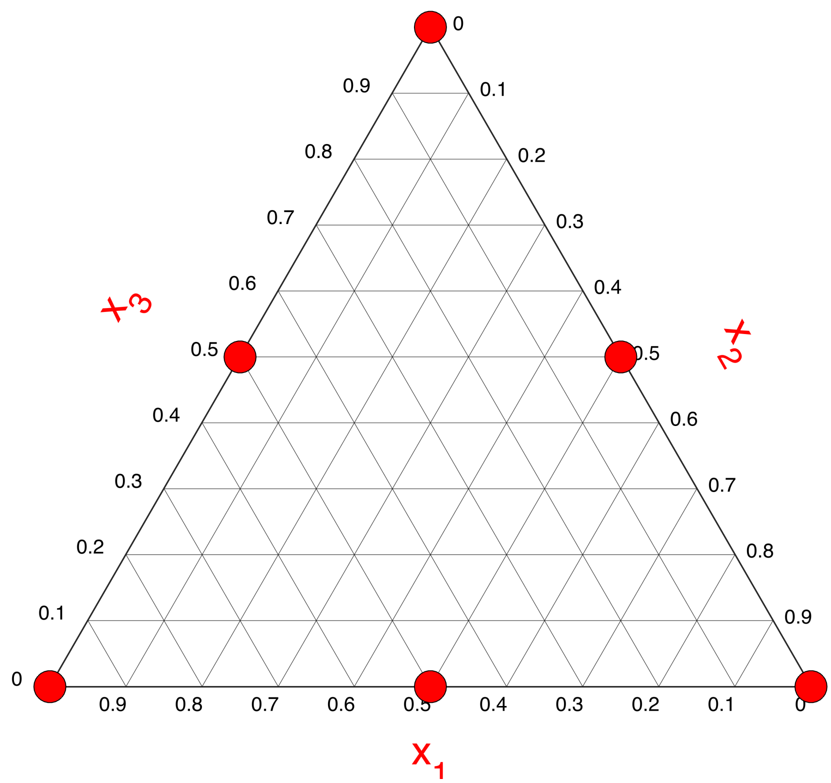
```
E=[0 0 1
    0 1 0
    1 0 0
    .5 .5 0
    .5 0 .5
    0 .5 .5];
disp(sym(E))
```

$$\begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \\ \frac{1}{2} & \frac{1}{2} & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & \frac{1}{2} & \frac{1}{2} \end{pmatrix}$$

Ternary diagram

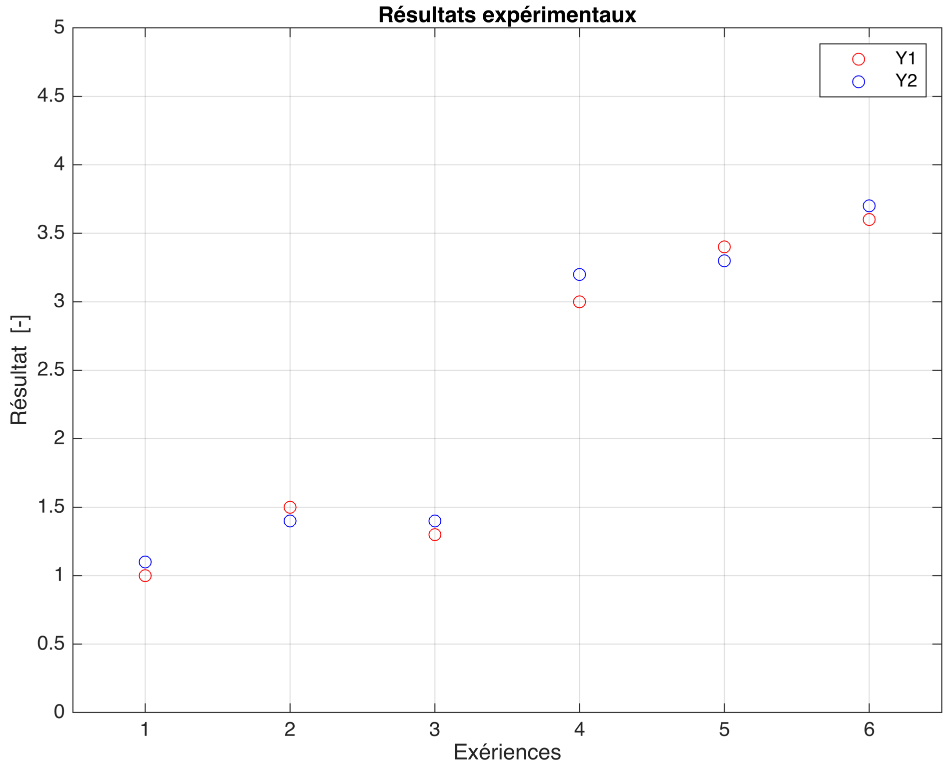
```
figure
h=ternplot(E(:,1),E(:,2),E(:,3),'ok');
set(h,'MarkerSize',16,'MarkerFaceColor','r')
h1=ternlabel('x_1','x_2','x_3');
```

```
set(h1(1),'FontSize',20,'Color','r','Position',[.5, -.1, 0])
set(h1(2),'FontSize',20,'Color','r','Position',[.9, .45, 0])
set(h1(3),'FontSize',20,'Color','r','Position',[.10, .5, 0])
```



Experimental data

```
Y1=[1;1.5;1.3;3;3.4;3.6];
Y2=[1.1;1.4;1.4;3.2;3.3;3.7];
figure
plot(1:6,Y1,'or',1:6,Y2,'ob')
title('Résultats expérimentaux')
xlabel('Exériences')
ylabel('Résultat  [-]')
legend('Y1','Y2')
grid on
axis([.5 6.5 0 5])
```



Fit

- The quadratic Scheffé's model is $y = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3$, therefore the matrix of the coefficients is:

```
spec=[1 0 0;0 1 0;0 0 1;1 1 0;1 0 1;0 1 1];
```

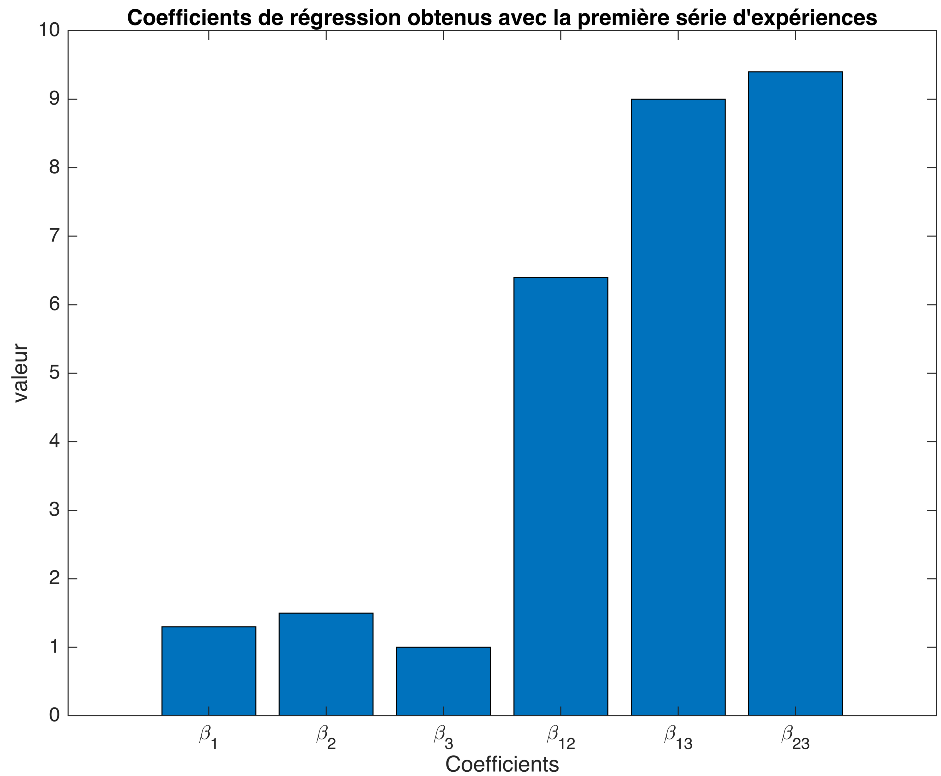
- The model matrix

```
X=x2fx(E,spec);
```

- The least square fit

```
beta=inv(X'*X)*X'*Y1;
labelcoef={'\beta_1' '\beta_2' '\beta_3' '\beta_{12}' '\beta_{13}'
'\beta_{23}'};
figure
bar(beta)
title('Coefficients de régression obtenus avec la première série
d''expériences')
xlabel('Coefficients')
```

```
ylabel('valeur')
set(gca,'XTickLabel',labelcoef)
```



We observe that the coefficients are positive. Second degree coefficients are much larger than linear coefficients.

Replicates

- Model fit

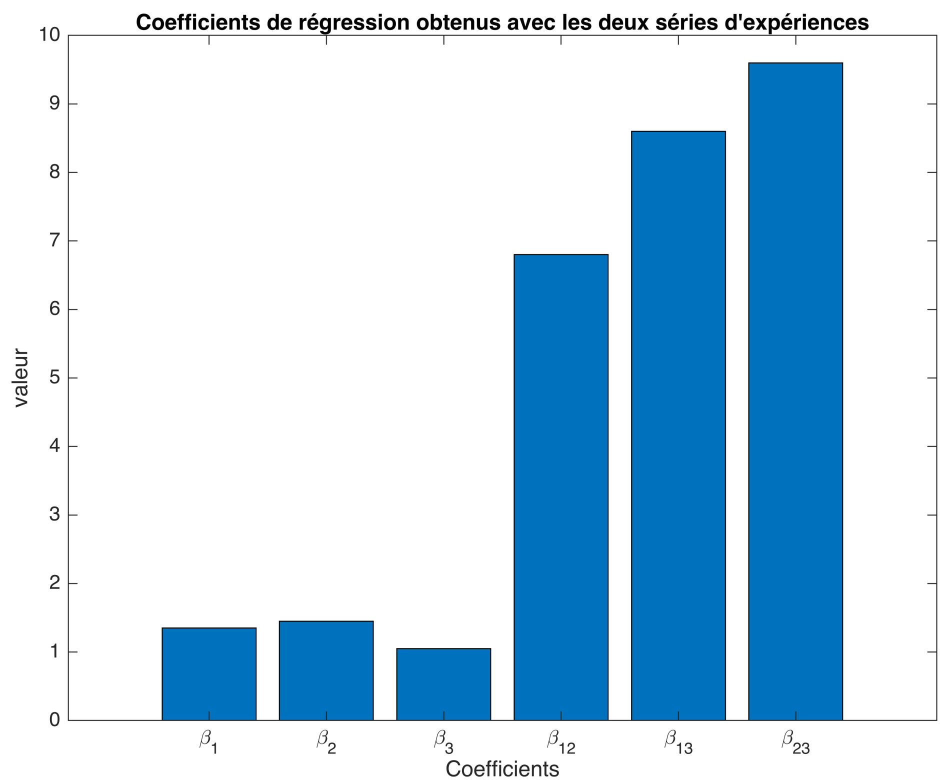
```
mdl=fitlm([E;E],[Y1;Y2],spec)
```

```
mdl =
Linear regression model:
    y ~ x1*x2 + x1*x3 + x2*x3

Estimated Coefficients:
             Estimate       SE        tStat       pValue  
             ________    ________    ______    __________

    x1         1.35      0.061237    22.045    5.6938e-07
    x2         1.45      0.061237    23.678    3.7244e-07
    x3         1.05      0.061237    17.146     2.519e-06
    x1:x2       6.8           0.3    22.667    4.8277e-07
    x1:x3       8.6           0.3    28.667    1.1933e-07
    x2:x3       9.6           0.3        32    6.1907e-08
```

```
Number of observations: 12, Error degrees of freedom: 6
Root Mean Squared Error: 0.0866
```

- *Barchart* of the coefficients

```
figure
bar(mdl.Coefficients.Estimate)
title('Coefficients de régression obtenus avec les deux séries
d''expériences')
xlabel('Coefficients')
ylabel('valeur')
set(gca,'XTickLabel',labelcoef)
```



Anova

We observe that all the coefficients are significant. On the other hand, there is no way with the plan used to determine a lack of fit since there are 6 experience points and 6 coefficients.

```
anova(mdl)
```

ans = 7×5 table

	SumSq	DF	MeanSq	F	pValue
1 x1	16.8070	1	16.8070	2.2409e+03	0
2 x2	19.2413	1	19.2413	2.5655e+03	0

	SumSq	DF	MeanSq	F	pValue
3 x3	15.4630	1	15.4630	2.0617e+03	0
4 x1:x2	3.8533	1	3.8533	513.7778	0
5 x1:x3	6.1633	1	6.1633	821.7778	0
6 x2:x3	7.6800	1	7.6800	1.0240e+03	0
7 Error	0.0450	6	0.0075	1	0.5000

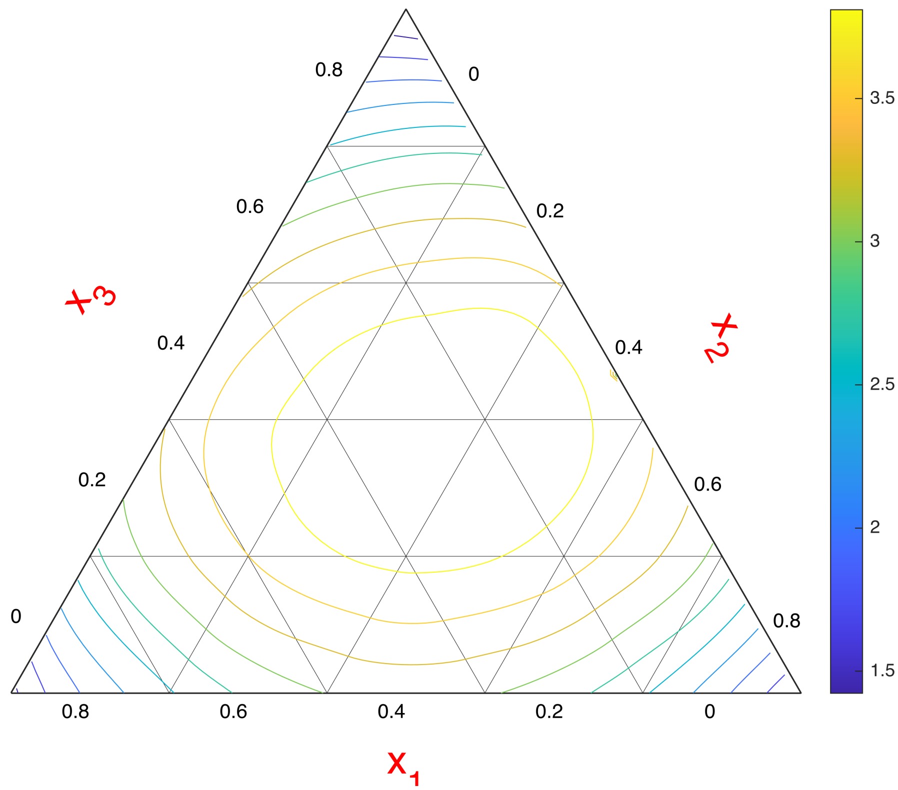
Surface response

Generating a 6-level simplex to estimate the function on the triangular surface

```
S5=(fullfact([6 6 6])-1)/5;
index=sum(S5,2)==1;
S5=S5(index,:);
X5=x2fx(S5,spec);
```

- Contour lines

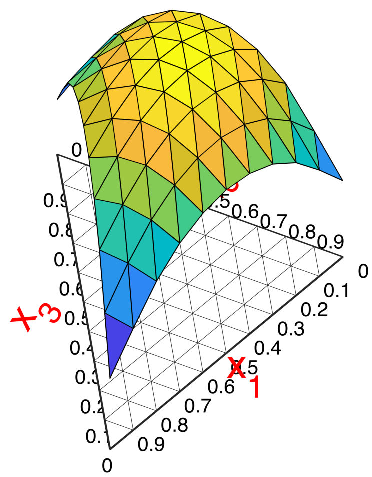
```
figure
terncontour(S5(:,1),S5(:,2),S5(:,3),X5*mdl.Coefficients.Estimate)
colorbar

h1=ternlabel('x_1','x_2','x_3');
set(h1(1),'FontSize',20,'Color','r','Position',[.5, -.1, 0])
set(h1(2),'FontSize',20,'Color','r','Position',[.9, .45, 0])
set(h1(3),'FontSize',20,'Color','r','Position',[.10, .5, 0])
```



On the graph above, the scales of the axes are are invered!

- 3D surface

```
%figure
ternsurf(S5(:,1),S5(:,2),S5(:,3),X5*mdl.Coefficients.Estimate);
h1=ternlabel('x_1','x_2','x_3');
set(h1(1),'FontSize',20,'Color','r','Position',[.5, -.1, 0])
set(h1(2),'FontSize',20,'Color','r','Position',[.9, .45, 0])
set(h1(3),'FontSize',20,'Color','r','Position',[.10, .5, 0])
view(-40,80)
```




```
Warning: Graphics timeout occurred. To share details of this issue with MathWorks technical
support, please include that this is an unresponsive graphics client with your service request.
```

It can be observed with these surfaces that the combinations which give the maximum responses are located between the center of the simplex and the right edge, therefore for concentrations of which are around 40%, the two other products remaining with close concentrations.