

Experiments plannification

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```
clear;
close all;
clc
addpath('./modules')
```

Global variables definition

```
global nb_cath
global name_elements
global do_not_align
global optimize_price_box
global impose_alignments_name
global impose_alignments_index
global not_repeat
global repeat_only
global repeat_at_least
global impose_plane_name
global impose_plane_index
global state
global f_plane_set
global nb_draw
global nb_draws_tot
global f_gradient_set
global path
global subfolder
global mixture_name_list
global mixture_list

state="run";
```

STOP button: to kill program whenever it is needed

```
fig_stop_button=figure;
set(fig_stop_button, 'Position', get(fig_stop_button, 'Position').*[1 1 0 0] + [-100 0 100 80]);
stop_button = uicontrol ( fig_stop_button , 'style' , ' pushbutton' , 'position', [35 35 60 30] , 'string' , 'STOP ' , 'cal
```



GUI for user to input the elements and number of cathodes

```
fig1 = figure ;
set(fig1, 'Position', get(fig1, 'Position').*[1 1 0 0] + [0 -250 150 350]);

uicontrol ( fig1 , 'style' , ' text' , 'position', [35 300 100 30] , 'string' , 'Number of cathodes ' );
for nc=2:3
```

```

nb_cathodes(nc-1) = uicontrol ( fig1 , 'style' , ' checkbox' , 'position', [3+30*nc,290,50,20] , 'Max' , 1 , 'string'
end
uicontrol ( fig1 , 'style' , ' text' , 'position', [55 250 60 30] , 'string' , 'Elements ' );
for i=1:7
    elements(i) = uicontrol ( fig1 , 'style' , ' edit' , 'position', [60,250-i*20,50,20] , 'Max' , 1 , 'string' , '' );
end
valid_elements_button=uicontrol ( fig1 , 'style' , 'push' , 'position' , [30 50 100 30 ] , 'string' , 'Elements validation'
uiwait(fig1);

```

```

name_elements = 105 string array
"A"      "B"      "C"      "D"      "E"

```

Get the elements and number of cathodes

If the user did not chose the number of cathode, error message is printed

```

nb_elements=size(name_elements,2);
nb_cath_box=get(nb_cathodes,'Value');
if nb_cath_box{1}==[1]
    nb_cath=2;
elseif nb_cath_box{2}==[1]
    nb_cath=3;
else
    fig_5 = figure ;
    set( fig_5 , 'position' , get(fig1,'Position').*[1 1 0 0] + [0 -50 400 75]);
    uicontrol ( fig_5 , 'style' , ' text' , 'position', [30 30 300 30] , 'FontSize', 16, 'string' , 'No cathode !' );
    return
end

nb_type_mixture=nb_elements;

```

Compute coordinates of the Simplexe Centroid Mixture points and generate the names of the mixtures.

```

[mixture,name_mixture] = coordinates_name_centroid_points(nb_elements,name_elements);

mixture_name_list=[];
for i=1:nb_elements
    mixture_name_list=[mixture_name_list;name_mixture{i}]; % list of all mixture name of simplexe centroid design
end

mixture_list=[];
for i=1:nb_elements
    mixture_list=[mixture_list;mixture{i}]; % list of all mixture points coordinates of simplexe centroid design
end

```

Compute alignments / 1D gradients

```

[alignments,name_alignement]=compute_alignments(mixture,name_mixture, nb_elements);

```

```

fig2 = figure ;
set( fig2 , 'position' , get(fig1,'Position').*[1 1 0 0] + [0 -250 350 700]);

```

For 2 cathodes:

User selection conditions

```

if nb_cath==2
    uicontrol ( fig2 , 'style' , ' text' , 'position', [60 660 240 30] , 'string' , 'Optimize price and number of experime
    optimize_price_box= uicontrol ( fig2 , 'style' , ' checkbox' , 'position', [40,675,15,15] ) ;

```

```

for i=1:size(name_alignment)
    list_alignment(i)=[name_alignment(i,1)+"-"+name_alignment(i,2)+"-"+name_alignment(i,3)];
end
uicontrol ( fig2 , 'style' , ' text' , 'position', [50 630 100 30] , 'string' , 'Impose alignments: ' );
list_align_impose=uicontrol ( fig2 , 'style' , 'listbox' , 'position', [50 540 200 100] , 'Max',size(name_alignment,1)

uicontrol ( fig2 , 'style' , ' text' , 'position', [25 500 100 30] , 'string' , 'Not repeat: ' );
not_repeat_list=uicontrol ( fig2 , 'style' , 'listbox' , 'position', [50 410 200 100] , 'Max',size(mixture_name_list,1)

uicontrol ( fig2 , 'style' , ' text' , 'position', [35 370 100 30] , 'string' , 'Repeat only: ' );
repeat_only_list=uicontrol ( fig2 , 'style' , 'listbox' , 'position', [50 280 70 100] , 'Max',size(mixture_name_list,1)
number_repet_only=[];
fix_repetition_only_button=uicontrol ( fig2 , 'style' , 'push' , 'position' , [120 300 100 50 ] , 'string' , '<html>Max

uicontrol ( fig2 , 'style' , ' text' , 'position', [40 240 100 30] , 'string' , 'Repeat at least: ' )
repeat_at_least_list=uicontrol ( fig2 , 'style' , 'listbox' , 'position', [50 150 70 100] , 'Max',size(mixture_name_list,1)
number_repeat_at_least=[];
fix_repetition_at_least_button=uicontrol ( fig2 , 'style' , 'push' , 'position' , [120 175 100 50 ] , 'string' , '<html>Max

uicontrol ( fig2 , 'style' , ' text' , 'position', [30 90 200 30] , 'string' , 'Do not align mixture of order: ' );
for da=1:nb_elements
    do_not_align_boxes(da)= uicontrol ( fig2 , 'style' , ' checkbox' , 'position', [50+da*30,75,50,20] , 'string' , 'no
end
valid_condition_button=uicontrol ( fig2 , 'style' , 'push' , 'position' , [100,40,50,20] , 'string' , 'Validation', 'cal

uiwait(fig2);

```

If user has ticked "Optimize price and number of experiments": GUI to input prices of all possible targets

```

if get(optimize_price_box,'Value')==1
    fig_price = figure ;
    nb_edit_per_line=0;
    div=10;
    % Compute number of boxes per lines to edit the window
    while nb_edit_per_line==0
        if mod((size(mixture_name_list,1)-1),div)==0
            nb_edit_per_line=div;
        else
            div=div-1;
        end
    end
    windows_height=(size(mixture_name_list,1)-1)/(nb_edit_per_line)*20+100;
    set( fig_price , 'position' , get(fig1,'Position').*[1 1 0 0] + [0 0 nb_edit_per_line*150 windows_height]);
    uicontrol ( fig_price , 'style' , ' text' , 'position', [20 windows_height-20 100 20] , 'string' , 'Target prices'
    for i=0:(size(mixture_name_list,1)-1)/(nb_edit_per_line)-1
        for j=1:nb_edit_per_line
            uicontrol ( fig_price , 'style' , ' text' , 'position', [20+(j-1)*130 windows_height-50-20*i 100 30] , 'string' , 'prices(i*nb_edit_per_line+j) = '
            prices(i*nb_edit_per_line+j) = uicontrol ( fig_price , 'style' , ' edit' , 'position', [100+(j-1)*130, windows_height-50-20*i 100 30] , 'string' , ''
        end
    end

    uicontrol ( fig_price , 'style' , ' text' , 'position', [20 30 200 30] , 'string' , 'or load prices list in csv, path= '
    path_prices=uicontrol ( fig_price , 'style' , ' edit' , 'position', [250 40 500 30] , 'string' , './ .csv' ) ;

    price_validation=uicontrol ( fig_price , 'style' , 'push' , 'position' , [120 10 50 20 ] , 'string' , 'OK', 'callback=@price_validation_callback'
    uiwait(fig_price);

```

Store prices in a list.

```

if get(path_prices,'string')~='./ .csv'
    table_prices=readtable(path_prices,'string')
    prices_list=[string(table2array(table_prices(:,1))),string(table2array(table_prices(:,2)))) ;
else
    prices_list=[mixture_name_list(1:end-1),get(prices,'string')];
end
end

```

Get user selection conditions

```

index_list_impose=get(list_align_impose,'Value');
index_not_repeat=get(not_repeat_list,'Value');
index_repeat_only=get(repeat_only_list,'Value');
if sum(index_repeat_only)>1
    str_nb_repeat_only= get(nb_repeat_only,'string');
    if length(index_repeat_only)==1
        number_repet_only=str2num(str_nb_repeat_only);
    else
        for i=1:length(index_repeat_only)
            number_repet_only(i)=str2num(str_nb_repeat_only{i});
        end
    end
end
end

```

```

index_repeat_at_least=get(repeat_at_least_list,'Value');
if sum(index_repeat_at_least)>1
    str_nb_repeat_at_least=get(nb_repeat_at_least,'string');
    if length(index_repeat_at_least)==1
        number_repeat_at_least=str2num(str_nb_repeat_at_least);
    else

        for i=1:length(index_repeat_at_least)
            number_repeat_at_least(i)=str2num(str_nb_repeat_at_least{i});
        end
    end

end

do_not_align_result=get(do_not_align_boxes,'Value');

```

Create lists containing :

- imposed alignments

```

impose_alignments_name = [];
impose_alignments_index=index_list_impose-1; % due to blank space left at the beginning of the listbox
for i=1:length(index_list_impose)
    if index_list_impose>1
        impose_alignments_name=[impose_alignments_name;name_alignement(index_list_impose(i)-1,:)];
    end
end

```

- mixtures to not repeat i.e. mixtures by which the final set of gradients should pass once and only once.

```

not_repeat=[];
for i=1:length(index_not_repeat)
    if index_not_repeat(i)>1
        not_repeat=[not_repeat;mixture_name_list(index_not_repeat(i)-1)];
    end
end

```

- mixtures to repeat only N times [mixture_name,N]

```

repeat_only=[];
for i=1:length(index_repeat_only)
    if index_repeat_only(i)>1
        repeat_only=[repeat_only;mixture_name_list(index_repeat_only(i)-1),number_repet_only(i)];
    end
end

```

- mixtures that should be repeated at least N times [mixture_name,N]

```

repeat_at_least=[];
for i=1:length(index_repeat_at_least)
    if index_repeat_at_least(i)>1
        repeat_at_least=[repeat_at_least;mixture_name_list(index_repeat_at_least(i)-1),number_repeat_at_least(i)];
    end
end

```

- mixture to not align i.e. that should not appear more than once in the same gradient: if pure elements should not be aligned, then the list is ['A','B','C',...]

```

do_not_align={};
for i=1:length(do_not_align_result)
    if do_not_align_result{i}==1
        do_not_align{end+1}=(name_mixture{i})';
    end
end

```

Compute a first 1D gradients set

```

nb_draw=0;
f_gradient_set=waitbar(0,"Compute gradient set: try number "+num2str(0));

if get(optimize_price_box,'Value')==0
    nb_draws_tot=1;
else
    nb_draws_tot=500;
end

[name_alignement_opt,alignement_opt] = gradients_set(name_mixture, mixture,alignments,name_alignement);
list_target = listing_targets(name_alignement_opt);
nb_alignments_best=size(name_alignement_opt,1)-1;

```

If user has ticked "Optimize price and number of experiments": we draw nb_draws set of gradients to keep the one with the lowest price / lowest number of gradients

```
if get(optimize_price_box,'Value')==1
```

Structures will store the set that minimizes the price among the nb_draw, and the set that minimizes the number of experiments among the nb_draw.

```
exp_opt=struct;  
price_opt=struct;
```

Initialize with the first set built before

```
price=price_calculation(prices_list,list_target(2:end));  
  
exp_opt.alignement_opt=alignement_opt;  
exp_opt.name_alignement_opt=name_alignement_opt;  
exp_opt.list_target=list_target;  
exp_opt.price=price;  
exp_opt.nb_alignments_best=nb_alignments_best;  
  
price_opt.alignement_opt=alignement_opt;  
price_opt.name_alignement_opt=name_alignement_opt;  
price_opt.list_target=list_target;  
price_opt.price=price;  
price_opt.nb_alignments_best=nb_alignments_best;
```

Make nb_draw sets of gradients to keep the best ones.

```
for i=1:nb_draws_tot-1  
  
    [name_alignement_opt_try,alignement_opt_try] = gradients_set(name_mixture, mixture,alignments,name_alignement)  
    list_target_try = listing_targets(name_alignement_opt_try);  
    price_try=price_calculation(prices_list,list_target_try(2:end));  
    nb_alignments_try=size(name_alignement_opt_try,1)-1;  
    if nb_alignments_try<exp_opt.nb_alignments_best  
        exp_opt.alignement_opt=alignement_opt_try;  
        exp_opt.name_alignement_opt=name_alignement_opt_try;  
        exp_opt.list_target=list_target_try;  
        exp_opt.price=price_try;  
        exp_opt.nb_alignments_best=nb_alignments_try;  
    end  
    if price_try<price_opt.price  
        price_opt.alignement_opt=alignement_opt_try;  
        price_opt.name_alignement_opt=name_alignement_opt_try;  
        price_opt.list_target=list_target_try;  
        price_opt.price=price_try;  
        price_opt.nb_alignments_best=nb_alignments_try;  
    end  
    nb_draw=i;  
end
```

Representation of the set of gradients

```
fig_representation_exp=plot_compo_space_gradients(nb_elements,mixture, name_mixture,name_elements, exp_opt.alignem  
title('Optimize number of experiments');  
fig_representation_price=plot_compo_space_gradients(nb_elements,mixture, name_mixture,name_elements, price_opt.ali  
title('Optimize price');  
fig_5=figure;  
height_fig5= size(price_opt.list_target,1)*30;  
set( fig_5 , 'position' , [ 800 , 300 ,400 , height_fig5 ] );  
uicontrol ( fig_5 , 'style' , ' text' , 'position', [10 height_fig5-40 200 30] , 'string' , 'List of targets: opt  
uicontrol ( fig_5 , 'style' , ' text' , 'position', [200 height_fig5-40 200 30] , 'string' , 'List of targets: op  
for i=1:size(price_opt.list_target,1)  
    uicontrol ( fig_5 , 'style' , ' text' , 'position', [20 height_fig5-40-20*i 200 30] , 'string' , price_opt.li  
end  
for i=1:size(exp_opt.list_target,1)  
    uicontrol ( fig_5 , 'style' , ' text' , 'position', [200 height_fig5-40-20*i 200 30] , 'string' , exp_opt.li  
end
```

Else if user has not ticked "Optimize price and number of experiments": we keep the first set and plot the gradients

```
else  
    fig_representation=plot_compo_space_gradients(nb_elements,mixture, name_mixture,name_elements, alignement_opt, 'b'  
    title('Set of experiments');  
    fig5=figure;  
    height_fig5= size(list_target,1)*20;  
    set( fig5 , 'position' , [ 800 , 300 ,200 , height_fig5 ] );  
    uicontrol ( fig5 , 'style' , ' text' , 'position', [10 height_fig5-40 200 30] , 'string' , 'List of targets' );  
    for i=1:size(list_target,1)  
        uicontrol ( fig5 , 'style' , ' text' , 'position', [20 height_fig5-40-20*i 200 30] , 'string' ,list_target(i)  
    end  
end  
end
```

☒ Optimize price and number of experiments

Impose alignments:

BC-ABCDE-ADE
BD-BCDE-CE
BD-ABCDE-ACE
BE-BCDE-CD
BE-ABCDE-ACD
CD-ABCDE-ABE
CE-ABCDE-ABD
DE-ABCDE-ABC

Not repeat:

E
AB
AC
AD
AE
BC
BD
BE

Repeat only:

A
B
C
D
E
AB
AC

Maximum number of repetitions >

A2
B2
C2
D2
E2

Repeat at least:

BDE
CDE
ABCD
ABCE
ABDE
ACDE
BCDE
ABCDE

Minimum number of repetitions >

ABCDE5

Do not align mixture of order:

☒ 1☐ 2☐ 3☐ 4☐ 5

Validation

```
nb_repeat_only =
  105 UIControl array:

  UIControl    UIControl    UIControl    UIControl    UIControl
nb_repeat_at_least =
  UIControl with properties:

    Style: 'edit'
    String: ''
    BackgroundColor: [0.9400 0.9400 0.9400]
    Callback: ''
    Value: 0
    Position: [290 240 50 20]
    Units: 'pixels'
```

Show all properties

Target prices

A	0	B	0	C	0	D	0	E	0	AB	0	AC	0	AD	0	AE	0	BC	0
BD	0	BE	0	CD	0	CE	0	DE	0	ABC	0	ABD	0	ABE	0	ACD	0	ACE	0
ADE	0	BCD	0	BCE	0	BDE	0	CDE	0	ABCD	0	ABCE	0	ABDE	0	ACDE	0	BODE	0

or load prices list in csv, path+name=

./prices_list.csv

OK

table_prices = 3002 table

	Var1	Var2
1	'A'	100
2	'B'	90
3	'C'	100
4	'D'	130
5	'E'	80
6	'AB'	190
7	'AC'	200
8	'AD'	230
9	'AE'	180
10	'BC'	190
11	'BD'	220
12	'BE'	170
13	'CD'	230
14	'DE'	210
15	'CE'	180
16	'ABC'	290
17	'ABD'	320
18	'ABE'	270
19	'ACD'	330
20	'ACE'	280
21	'ADE'	310

	Var1	Var2
22	'BCD'	320
23	'BCE'	270
24	'BDE'	300
25	'CDE'	310
26	'ABCD'	420
27	'ABCE'	370
28	'ABDE'	400
29	'ACDE'	410
30	'BCDE'	400

Compute gradient set: set number 498, try number 1

ans = 4
ans = 4

List of targets: optimize price

List of targets: optimize experiments

CD
ABE
CE
ABD
DE
ABC
BC
ADE
AE
BCD
E
AB
AC
BE
C
AD
BD
B
ACE
D
BCE
A
CDE

CD
ABE
CE
ABD
DE
ABC
AC
BDE
AD
BCE
D
AB
AE
BC
BD
ACE
C
BE
B
ACD
ADE
E
BCD
A
CDE

For 3 cathodes :

User selection conditions

```
if nb_cath==3
    [name_plane,plane] =compute_planes(name_alignement,alignments,nb_type_mixture);
```

Get user selection conditions

```
for i=1:size(name_plane)
    list_plane(i)=[name_plane(i,1)+"-"+name_plane(i,2)+"-"+name_plane(i,3)+"-"+name_plane(i,4)+"-"+name_plane(i,5)+"-"
end

uicontrol ( fig2 , 'style' , ' text' , 'position', [60 660 240 30] , 'string' , 'Optimize price and number of experime
optimize_price_box= uicontrol ( fig2 , 'style' , ' checkbox' , 'position', [40,675,15,15] ) ;

uicontrol ( fig2 , 'style' , ' text' , 'position', [50 630 100 30] , 'string' , 'Impose planes: ' );
list_plane_impose=uicontrol ( fig2 , 'style' , 'listbox' , 'position', [50 540 200 100] , 'Max',size(name_plane,1), 's

uicontrol ( fig2 , 'style' , ' text' , 'position', [50 500 100 30] , 'string' , 'Not repeat: ' );
not_repeat_list=uicontrol ( fig2 , 'style' , 'listbox' , 'position', [50 410 200 100] , 'Max',size(mixture_name_list,1
```

```

uicontrol ( fig2 , 'style' , ' text' , 'position', [50 370 100 30] , 'string' , 'Repeat only: ' );
repeat_only_list=uicontrol ( fig2 , 'style' , 'listbox' , 'position', [50 280 70 100] , 'Max',size(mixture_name_list,1
number_repet_only=[];
fix_repetition_only_button=uicontrol ( fig2 , 'style' , 'push' , 'position' , [120 300 100 50 ] , 'string' , '<html>Max

uicontrol ( fig2 , 'style' , ' text' , 'position', [40 240 100 30] , 'string' , 'Repeat at least: ' )
repeat_at_least_list=uicontrol ( fig2 , 'style' , 'listbox' , 'position', [50 150 70 100] , 'Max',size(mixture_name_li
number_repeat_at_least=[];
fix_repetition_at_least_button=uicontrol ( fig2 , 'style' , 'push' , 'position' , [120 175 100 50 ] , 'string' , '<html

valid_condition_button=uicontrol ( fig2 , 'style' , 'push' , 'position' , [150,100,50,20] , 'string' , 'Validation','ca

uiwait(fig2);

```

If user has ticked "Optimize price and number of experiments": GUI to input prices of all possible targets

```

if get(optimize_price_box,'Value')==1
    fig_price = figure ;
    nb_edit_per_line=0;
    div=10;
    while nb_edit_per_line==0
        if mod((size(mixture_name_list,1)-1),div)==0
            nb_edit_per_line=div;
        else
            div=div-1;
        end
    end
    windows_height=(size(mixture_name_list,1)-1)/(nb_edit_per_line)*20+100;
    set( fig_price , 'position' , get(fig1,'Position').*[1 1 0 0] + [0 0 nb_edit_per_line*150 windows_height]);
    uicontrol ( fig_price , 'style' , ' text' , 'position', [20 windows_height-20 100 20] , 'string' , 'Target prices'
    for i=0:(size(mixture_name_list,1)-1)/(nb_edit_per_line)-1
        for j=1:nb_edit_per_line
            uicontrol ( fig_price , 'style' , ' text' , 'position', [20+(j-1)*130 windows_height-50-20*i 100 30] , 'string' , mixture_name_list(i*nb_edit_per_line+j)
            prices(i*nb_edit_per_line+j) = uicontrol ( fig_price , 'style' , ' edit' , 'position', [100+(j-1)*130, windows_height-50-20*i 100 30] , 'string' , ''
        end
    end

    fix_repetition_at_least_button=uicontrol ( fig_price , 'style' , 'push' , 'position' , [120 20 50 20 ] , 'string' , 'Fix repetition at least'
    uiwait(fig_price)
end

```

Store prices in a list.

```

prices_list=[mixture_name_list(1:end-1),get(prices,'string')];

index_list_impose=get(list_plane_impose,'Value');
index_not_repeat=get(not_repeat_list,'Value');
index_repeat_only=get(repeat_only_list,'Value');
if sum(index_repeat_only)>1
    str_nb_repeat_only= get(nb_repet_only,'string');
    if length(index_repeat_only)==1
        number_repeat_only=str2num(str_nb_repeat_only);
    else
        for i=1:length(index_repeat_only)
            number_repeat_only(i)=str2num(str_nb_repeat_only{i});
        end
    end
end

index_repeat_at_least=get(repeat_at_least_list,'Value');
if sum(index_repeat_at_least)>1
    str_nb_repet_at_least=get(nb_repet_at_least,'string');
    if length(index_repeat_at_least)==1
        number_repeat_at_least=str2num(str_nb_repet_at_least);
    else
        for i=1:length(index_repeat_at_least)
            number_repeat_at_least(i)=str2num(str_nb_repet_at_least{i});
        end
    end
end
end

```

Create lists containing :

- imposed planes

```

impose_plane_name =[];
impose_plane_index=index_list_impose-1;
for i=1:length(index_list_impose)
    if index_list_impose>1
        impose_plane_name=[impose_plane_name;name_plane(index_list_impose(i)-1,:)];
    end
end

```


- mixtures to not repeat i.e. mixtures by which the final set of gradients should pass once and only once.

```
not_repeat=[];
for i=1:length(index_not_repeat)
    if index_not_repeat(i)>1
        not_repeat=[not_repeat;mixture_name_list(index_not_repeat(i)-1)];
    end
end
```

- mixtures to repeat only N times [mixture_name,N]

```
repeat_only=[];
for i=1:length(index_repeat_only)
    if index_repeat_only(i)>1
        repeat_only=[repeat_only;mixture_name_list(index_repeat_only(i)-1),number_repet_only(i)];
    end
end
```

- mixtures to repeat at least N times [mixture_name,N]

```
repeat_at_least=[];
for i=1:length(index_repeat_at_least)
    if index_repeat_at_least(i)>1
        repeat_at_least=[repeat_at_least;mixture_name_list(index_repeat_at_least(i)-1),number_repeat_at_least(i)];
    end
end
```

NB: no condition such as "do_not_align" because the planes encompass 7 points and such conditions would lead to no solution

Compute a first 2D planes set

```
nb_draw=0;
f_plane_set=waitbar(0,"Compute planes set: try number "+num2str(0));
if get(optimize_price_box,'Value')==0
    nb_draws_tot=1;
else
    nb_draws_tot=500;
end
[name_plane_opt,plane_opt] = planes_set(name_mixture, mixture,plane,name_plane);
list_target = listing_targets_3cath(name_plane_opt);
nb_planes_best=size(name_plane_opt,1)-1;
```

If user has ticked "Optimize price and number of experiments": we draw nb_draws set of planes to keep the one with the lowest price / lowest number of planes

```
if get(optimize_price_box,'Value')==1
```

Structures will store the set that minimizes the price among the nb_draw, and the set that minimizes the number of experiments among the nb_draw.

```
exp_opt=struct;
price_opt=struct;
price=price_calculation(prices_list,list_target(2:end));
```

Initialize with the first set built before

```
exp_opt.plane_opt=plane_opt;
exp_opt.name_plane_opt=name_plane_opt;
exp_opt.list_target=list_target;
exp_opt.price=price;
exp_opt.nb_planes_best=nb_planes_best;

price_opt.plane_opt=plane_opt;
price_opt.name_plane_opt=name_plane_opt;
price_opt.list_target=list_target;
price_opt.price=price;
price_opt.nb_planes_best=nb_planes_best;
```

Make nb_draw sets of planes to keep the best ones.

```
for i=1: nb_draws_tot-1
    [name_plane_opt_try,plane_opt_try] = planes_set(name_mixture, mixture,plane,name_plane);
    list_target_try = listing_targets_3cath(name_plane_opt_try);
    price_try=price_calculation(prices_list,list_target_try(2:end));
    nb_planes_try=size(name_plane_opt_try,1)-1;
    if nb_planes_try<exp_opt.nb_planes_best
        exp_opt.plane_opt=plane_opt_try;
        exp_opt.name_plane_opt=name_plane_opt_try;
        exp_opt.list_target=list_target_try;
        exp_opt.price=price_try;
        exp_opt.nb_planes_best=nb_planes_try;
    end
    if price_try<price_opt.price
        price_opt.plane_opt=plane_opt_try;
        price_opt.name_plane_opt=name_plane_opt_try;
```

```

        price_opt.list_target=list_target_try;
        price_opt.price=price_try;
        price_opt.nb_planes_best=nb_planes_try;
    end
    nb_draw=i
end

```

Representation of the set of planes

```

fig_representation_exp=plot_compo_space_planes(nb_elements,mixture, name_mixture,name_elements,exp_opt.plane_opt,
title('Optimize number of experiments'))
fig_representation_price=plot_compo_space_planes(nb_elements,mixture, name_mixture,name_elements,price_opt.plane_o
title('Optimize price'));

fig_5=figure;
height_fig5= size(price_opt.list_target,1)*30;
set( fig_5 , 'position' , [ 800 , 300 ,400 , height_fig5 ] );
uicontrol ( fig_5 , 'style' , ' text' , 'position', [10 height_fig5-40 200 30] , 'string' , 'List of targets: opt
uicontrol ( fig_5 , 'style' , ' text' , 'position', [200 height_fig5-40 200 30] , 'string' , 'List of targets: op

for i=1:size(price_opt.list_target,1)
    uicontrol ( fig_5 , 'style' , ' text' , 'position', [20 height_fig5-40-20*i 200 30] , 'string' , price_opt.li
end
for i=1:size(exp_opt.list_target,1)
    uicontrol ( fig_5 , 'style' , ' text' , 'position', [200 height_fig5-40-20*i 200 30] , 'string' , exp_opt.lis
end

```

Else if user has not ticked "Optimize price and number of experiments": we keep the first set and plot the planes

```

else
    fig_representation=plot_compo_space_planes(nb_elements,mixture, name_mixture,name_elements,plane_opt, 'r',3 );
    title('Set of planes');

    fig5=figure;
    height_fig5= size(list_target,1)*20;
    set( fig5 , 'position' , [ 800 , 300 ,200 , height_fig5 ] );
    uicontrol ( fig5 , 'style' , ' text' , 'position', [10 height_fig5-40 200 30] , 'string' , 'List of targets' );

    for i=1:size(list_target,1)
        uicontrol ( fig5 , 'style' , ' text' , 'position', [20 height_fig5-40-20*i 200 30] , 'string' ,list_target(i)
    end

end

end

```

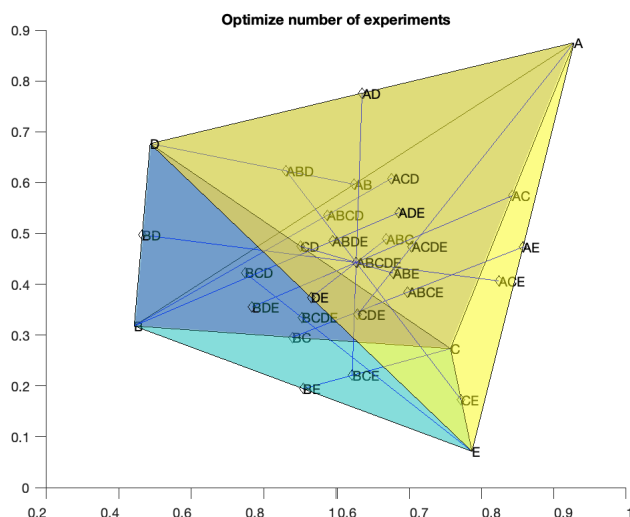
Save the set of gradients/planes and user condition for the draw

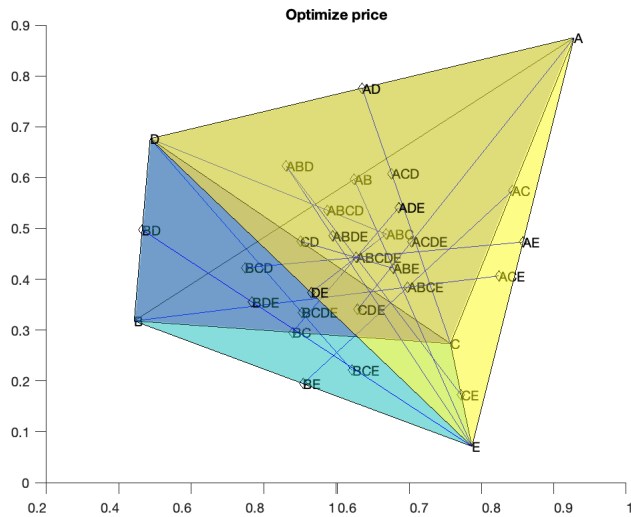
GUI for input the path for save

```

fig_sortie=figure;
set(fig_sortie,'Position', get(fig_sortie,'Position').*[1 1 0 0] + [0 0 600 100]);
uicontrol ( fig_sortie , 'style' , ' text' , 'position', [20 70 100 30] , 'string' , 'Save path ' );
save=uicontrol ( fig_sortie , 'style' , ' edit' , 'position', [20 40 500 30] , 'string' , './' ) ;
button_save=uicontrol ( fig_sortie , 'style' , ' push' , 'position', [20 10 40 20] , 'string' , 'Save ' , 'callback', 'uire
uiwait(fig_sortie);

```





Save path

Save

Save result

```
path=get(save, 'String');
parameters_file()
```

If price and number of experiments were optimized

Save targets list

```
if get(optimize_price_box, 'Value')==1
    writematrix(["List of targets";exp_opt.list_target],path+subfolder+"/Target_list_optimize_nb_experiments.csv");
    writematrix(["List of targets";exp_opt.list_target],path+subfolder+"/Target_list_optimize_price_experiments.csv");
    writematrix(["List of possible targets","Price";prices_list],path+subfolder+"/Target price list.csv");
```

Save the representation of composition space and set of gradients/planes

```
savefig(fig_representation_exp,path+subfolder+"/Representation_experiments_optimize_nb_experiments.fig");
savefig(fig_representation_price,path+subfolder+"/Representation_experiments_optimize_price_experiments.fig");
if nb_cath==2
    writematrix(["Target 1","gradient center","Target 2"; price_opt.name_alignement_opt(2:end,:)], path+subfolder+"/Ex
    writematrix(["Target 1","gradient center","Target 2";exp_opt.name_alignement_opt(2:end,:)], path+subfolder+"/Exper
end

if nb_cath==3
    writematrix(["Target 1","gradient center","Target 2","gradient center","Target 3","gradient center","plane center"
    writematrix(exp_opt.name_plane_opt(2:end,:), path+subfolder+"/Experimental_plane_optimize_nb_experiments.csv");
end
```

If price and number of experiments were not optimized

```
else
    writematrix(["List of targets";list_target(2:end,:)],path+subfolder+"/Target_list.csv");
    savefig(fig_representation,path+subfolder+"/Representation_experiments.fig");
    if nb_cath==2
        writematrix(["Target 1","gradient center","Target 2";name_alignement_opt(2:end,:)], path+subfolder+"/Experimental_
    end

    if nb_cath==3
        writematrix(["Target 1","gradient center","Target 2","gradient center","Target 3","gradient center","plane center"
    end
end
```

Display message to user

```
fig_success=figure;
set( fig_success , 'position' , get(fig_success,'Position').*[1 1 0 0] + [0 -50 500 75]);
uicontrol ( fig_success , 'style' , ' text' , 'position' , [30 30 400 30] , 'FontSize' , 16,'string' , 'Try was saved su
```

Try was saved successfully

