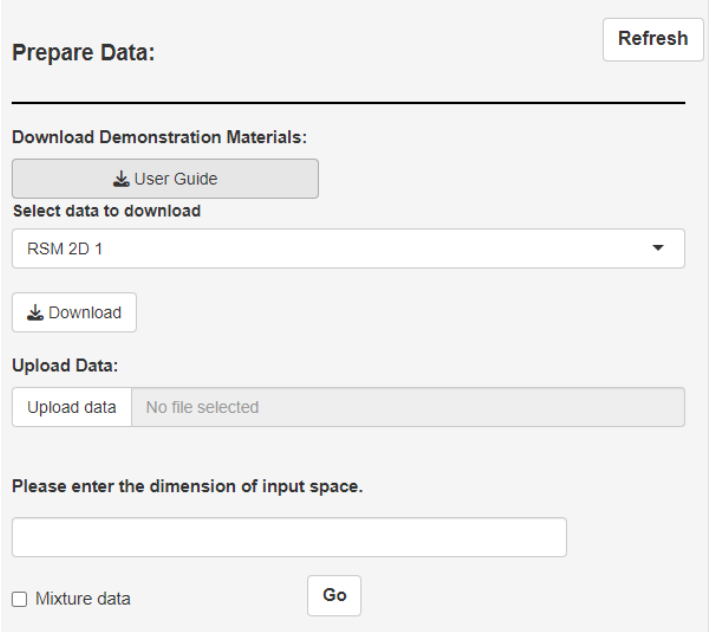
Quick Non-Uniform Space Filling (QNUSF) Designs Application User Guide

Xiankui Yang, University of South Florida, Tampa, FL
Lu Lu, University of South Florida, Tampa, FL
Christine M. Anderson-Cook, Los Alamos, NM

This guide will direct you through the steps needed to construct a QNUSF design of the dimension and run size required for your experiment. There are two ways to access this app. The first is the web version accessible via this link: https://xiankuiyangstatistics.shinyapps.io/QNUSF/. The second is the desktop version that can be downloaded from GitHub at the link: https://github.com/XiankuiYang/QNUSF, and run locally in R Shiny. Note there is a memory usage limitation of 1 GB for the web version. The desktop version will allow the users to work with larger datasets depending on the available RAM of your local computer.

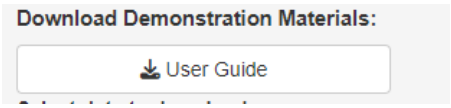
Section 1: Data Preparation

Section 1.1: Prepare Data – The dialog box below shows the Prepare Data section which provides information needed to construct the design from a candidate set of possible design locations with user assigned weights.

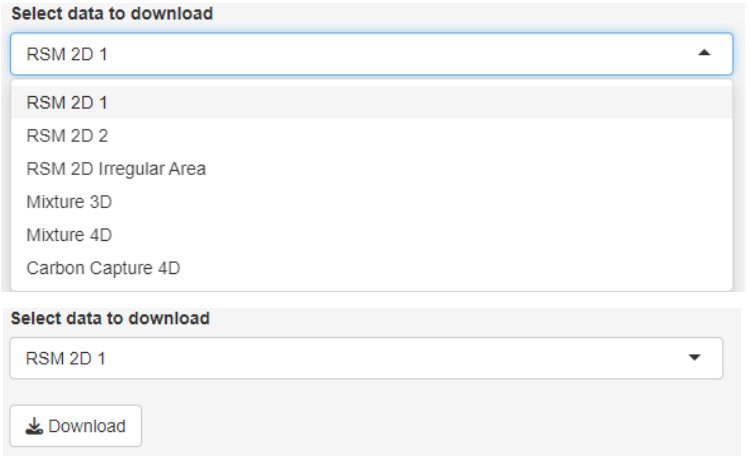


- In the ***Prepare Data*** section, upload a candidate data set from which the QNUSF design will be constructed. To start constructing a new design, click "**Refresh**" button to remove any historical designs or data sets that have been previously entered.

Section 1.1.1: Download Reference Materials and Sample Candidate Data Sets



- You may download this guide by clicking the "***User Guide***" button

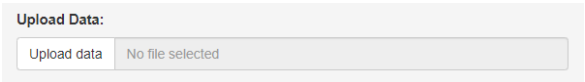


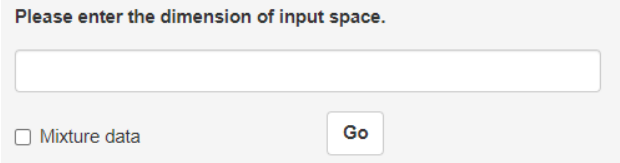
- To use an existing example, download one of the sample candidate data sets by selecting the data you want and then clicking "***Download***" button. The example below shows the first few rows with the format for the candidate data, with the initial columns defining locations in the design region of interest, and the final column assigning a weight to that candidate design point.

	A	B	C	D
1	X1	X2	X3	Weight
2	-1	-1	-1	25.49067
3	-1	-1	-0.875	27.00822
4	-1	-1	-0.75	28.36752
5	-1	-1	-0.625	29.56855
6	-1	-1	-0.5	30.61133
7	-1	-1	-0.375	31.49584
8	-1	-1	-0.25	32.22209
9	-1	-1	-0.125	32.79008
10	-1	-1	0	33.19981
11	-1	-1	0.125	33.45127
12	-1	-1	0.25	33.54448
13	-1	-1	0.375	33.47943
14	-1	-1	0.5	33.25611

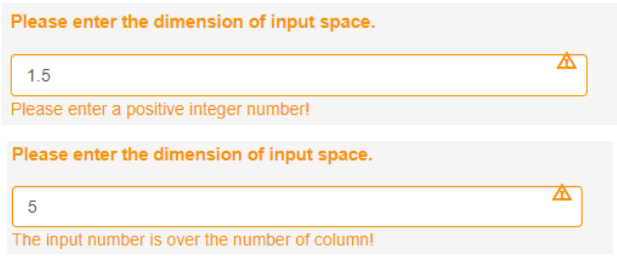
Section 1.1.2: Upload Data

- To begin constructing a QNUSF design, click the ***Upload data*** button to upload a .csv file with your candidate data set. Ensure that the data has the appropriate format with the first ***n*** columns contain the ***n***-dimensional input locations, and the last column contains **user assigned** weights.





- After the data set is uploaded, enter the dimension of input space for the design to be constructed. The dimension should be an integer ≥1. This is required by the app to process the candidate data set provided.
- If the data is a mixture data, click the check box "***Mixture data***". After all the above is done, click the "***Go***" button. If there are any errors with the dimension of the input space or the .csv file, warning messages will be generated.



If there are no problems with the inputs, then the application will populate the ***Data Visualization*** tab.

Section 1.2: Visualize Data

Section 1.2.1: Data Visualization

- After clicking the "***Go***" button, a new tab called ***Data Visualization*** is created.

- The first portion of the display shows a table of the provided candidate set. You can specify the number of top rows from the candidate set to display by entering a value in the ***Rows* textbox**. The default number is "**5**". You can also select the number of rows to display per page in the ***Show Entries*** textbox. For example, if you set the number of entries to 10, the table will show 10 rows per page. If you choose to display the top 100 rows and show 10 rows per page, then the table will have 10 total pages, and you can navigate through the pages using the page selector located at the bottom right of the table to view all the sample candidate points.

Rows

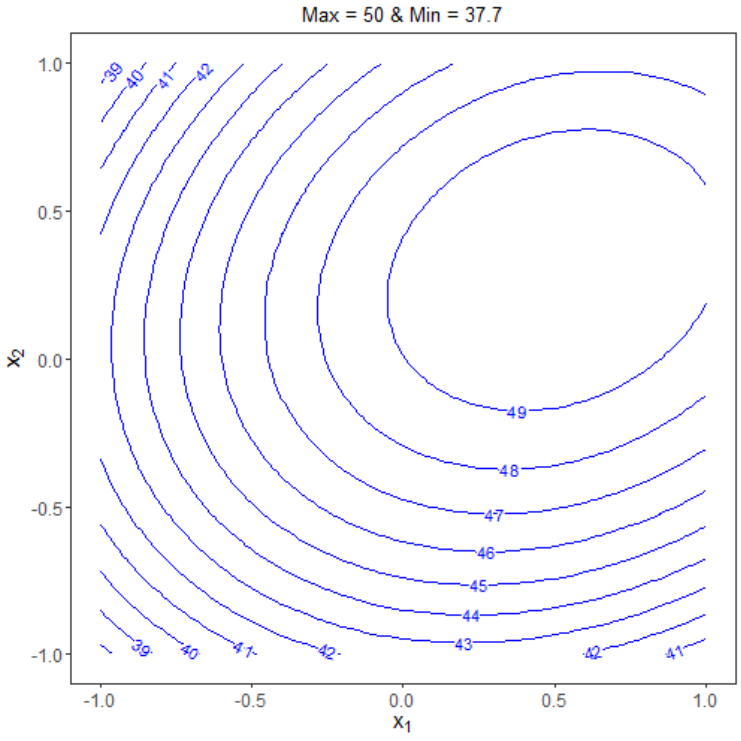
100

Show 10 entries

	X1	X2	X3	Weight
1	-1	-1	-1	25.491
2	-1	-1	-0.875	27.008
3	-1	-1	-0.75	28.368
4	-1	-1	-0.625	29.569
5	-1	-1	-0.5	30.611
6	-1	-1	-0.375	31.496
7	-1	-1	-0.25	32.222
8	-1	-1	-0.125	32.79
9	-1	-1	0	33.2
10	-1	-1	0.125	33.451

Previous 1 2 3 4 5 … 10 Next

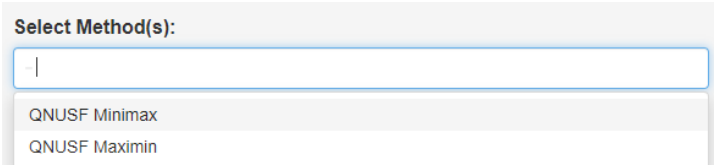
- The second portion of the display includes available plots (for special dimensional cases). The plots show contour plots of the weights throughout the specified input space. These can be used to verify that the candidate set entered matches what was intended. The plots are available for lower dimensional cases (1D, 2D, and 3D RSM data; 3D and 4D mixture data). A sample plot for a 2D example is shown below.



Section 2: Creating QNUSF Designs

In this phase, a design is constructed using the provided candidate set. The user can specify the type of design as well as the number of runs.

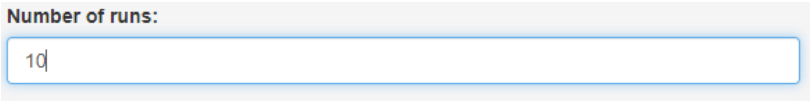
- The first choice for the user is to identify the type of design to be constructed. This is done through the Select Method(s) drop-down menu. There are two choices:
    - Minimax – this minimizes the maximum distance between any point in the candidate set and the nearest design point.
    - Maximin – this maximizes the minimum distance between any two design points.



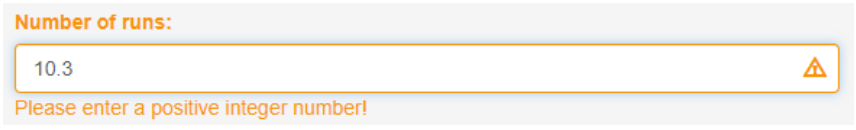
Note: 1. Minimax designs tend to not put as many designs close to the edges of the design space (as specified by the candidate set) as Maximin designs which tend to push selected design points to the edges of the design space.

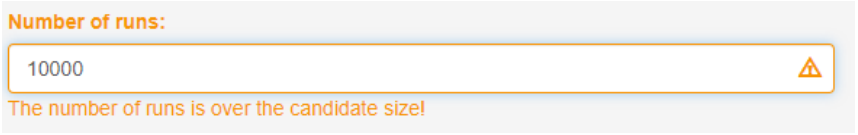
2. You can choose one or both of the Minimax and Maximin options, by highlighting those choices.

- Next, specify a positive integer for the ***Number of runs*** textbox. The default number is "**10**". This number cannot be larger than the size of the candidate set.



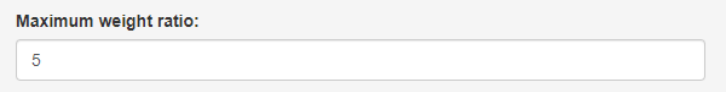
- If a number is not a positive integer number or larger than the candidate set size, a warning message appears in orange.



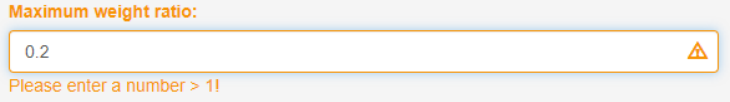


- Next specify the ***Maximum weight ratio*** value in the textbox. Acceptable values are real numbers greater than or equal to 1. The choice of this value specifies the range of scaled weights that will be used to generate the design. All weights are scaled between 1 and the selected maximum weight

ratio, with larger values corresponding to regions where the user wants a higher density of points in the design. The default number is "**5**". A value of 1 generates a uniform space filling design with equal emphasis in all regions of the design space. Larger values lead to designs with greater differences in concentrations of design points in different regions.



- If a number is less than 1, a warning message will appear in orange.



Note: We recommend creating multiple designs using both types of QNUSF designs (Minimax and Maximin) as well as different ***Maximum weight ratio*** values to compare alternatives and find the best match to the experimental needs of the study.

Section 2.1: Minimax Designs

- If you select ***QNUSF Minimax*** from the ***Select Method(s)*** menu, enter a number in the ***Number of runs*** textbox, and enter a number in the ***Maximum weight ratio*** textbox. Then click the ***Generate*** button to create a QNUSF Minimax distance design.

- After you click the ***Generate*** button, a new tab will appear, labelled ***Minimax***. Click on this tab to see the generated design shown in a ***Design Table***. The title shows which type of design was created, the number of runs in the design, and the selected maximum weight ratio. The ***Decimal*** textbox allows you to enter the desired precision of input locations (number of decimal places) for the resulting design. The "***Download***" button allows the created design to be saved as a .csv file. In the design table, we show the original weight values and scaled weight values (last column).
- If the dimension of the design allows for a contour plot to be generated (1D, 2D, and 3D RSM data or 3D and 4D mixture data), this plot will appear below the design table.

- The following figure shows a result for a 3-dimensional mixture data case. By right-clicking on the plot, you can save or copy the image.

Minimax, N=20, MWR=5

Design Table

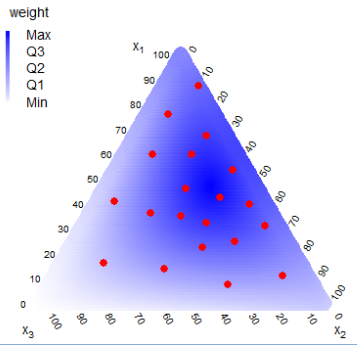
Decimal: 3

download

Show 10 entries

	x1	x2	x3	weight	Scaled Weight
1	0.425	0.425	0.15	1.729	4.955
2	0.537	0.412	0.05	1.674	4.874
3	0.462	0.288	0.25	1.642	4.828
4	0.6	0.238	0.162	1.633	4.815
5	0.675	0.25	0.075	1.617	4.792
6	0.4	0.537	0.062	1.56	4.71
7	0.325	0.425	0.25	1.56	4.709
8	0.35	0.325	0.325	1.478	4.591
9	0.25	0.562	0.188	1.337	4.386
10	0.312	0.637	0.05	1.328	4.374

Previous 1 2 Next



Section 2.2: Maximin Designs

- If you select ***QNUSF Maximin*** from the ***Select Method(s)*** menu, enter a number in the ***Number of runs*** textbox, and enter a number in the ***Maximum weight ratio*** textbox. Then click the ***Generate*** button to create a QNUSF Maximin distance design.

- After you click the ***Generate*** button, a new tab will appear, labelled ***Maximin***. Click on this tab to see the generated design shown in a ***Design Table***. The title shows which type of design was created, the number of runs in the design, and the selected maximum weight ratio. The ***Decimal*** textbox allows you to enter the desired precision of input locations (number of decimal places) for the resulting design. The "***Download***" button allows the created design to be saved as a .csv file. In the design table, we show both the original weight values and scaled weight values (last column).
- If the dimension of the design allows for a contour plot to be generated (1D, 2D, and 3D RSM data or 3D and 4D mixture data), this plot will appear below the design table.
- The following figure shows a result for a 3-dimensional mixture data case. By right-clicking on the plot, you can save or copy the image.

Maximin, N=20, MWR=5

Design Table

Decimal

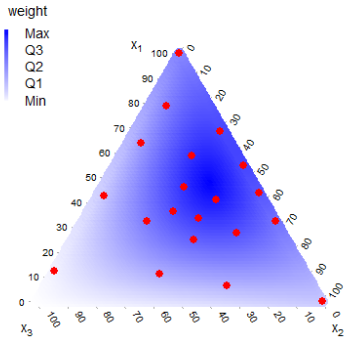
3

download

Show 10 entries

	x1	x2	x3	weight	Scaled Weight
1	0.412	0.425	0.162	1.72	4.942
2	0.588	0.25	0.162	1.657	4.85
3	0.462	0.288	0.25	1.642	4.828
4	0.338	0.4	0.262	1.572	4.727
5	0.688	0.3	0.013	1.57	4.724
6	0.55	0.45	0	1.54	4.681
7	0.362	0.3	0.338	1.451	4.552
8	0.438	0.562	0	1.422	4.509
9	0.275	0.562	0.162	1.41	4.492
10	0.25	0.425	0.325	1.282	4.307

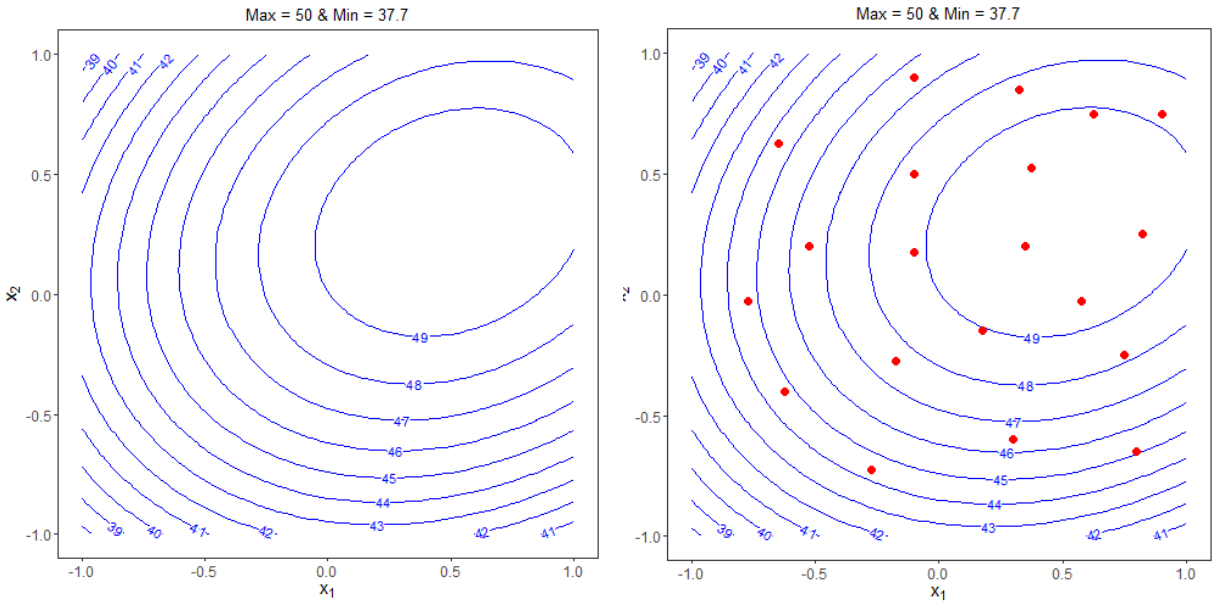
Previous 1 2 Next



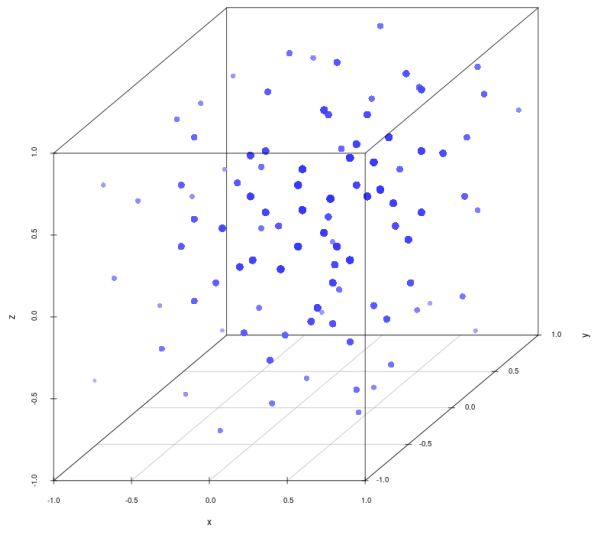
Section 3: Additional Information

Section 3.1: Description of available plots

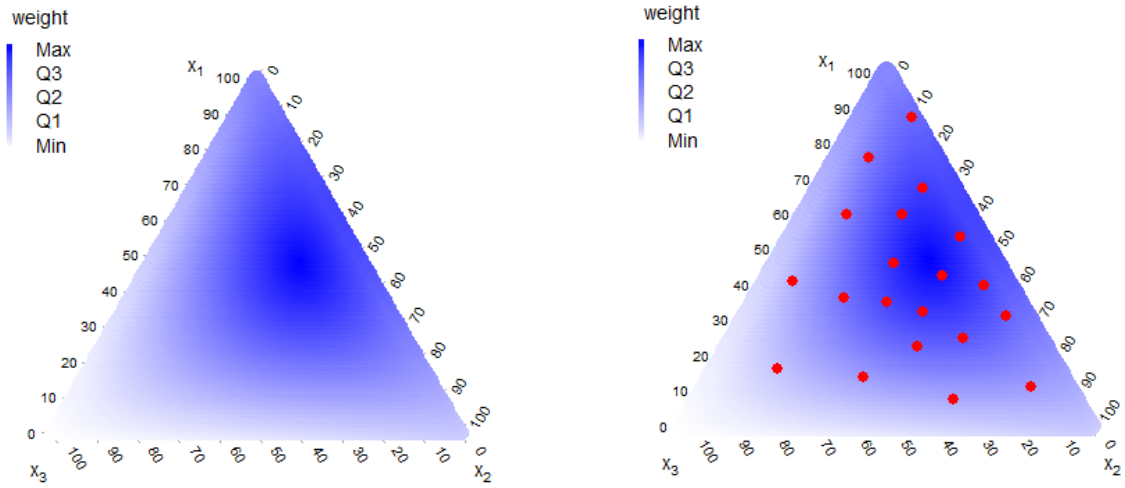
- For 2D RSM data, we use contour plot to summarize the weight distribution. The main title of the plot provides the information on the maximum and minimum values of the original weights in the candidate set. The plot automatically selects contour intervals to span the range of weights. The red points in plot on the right hand side represent the design points selected for the constructed design.



- For 3D RSM data, visualizing the weight distribution in 3D space can be challenging. To address this, we use a 3D scatter plot to display the design points along with their associated weight values. In this plot, larger point sizes and darker blue color indicate higher weights.

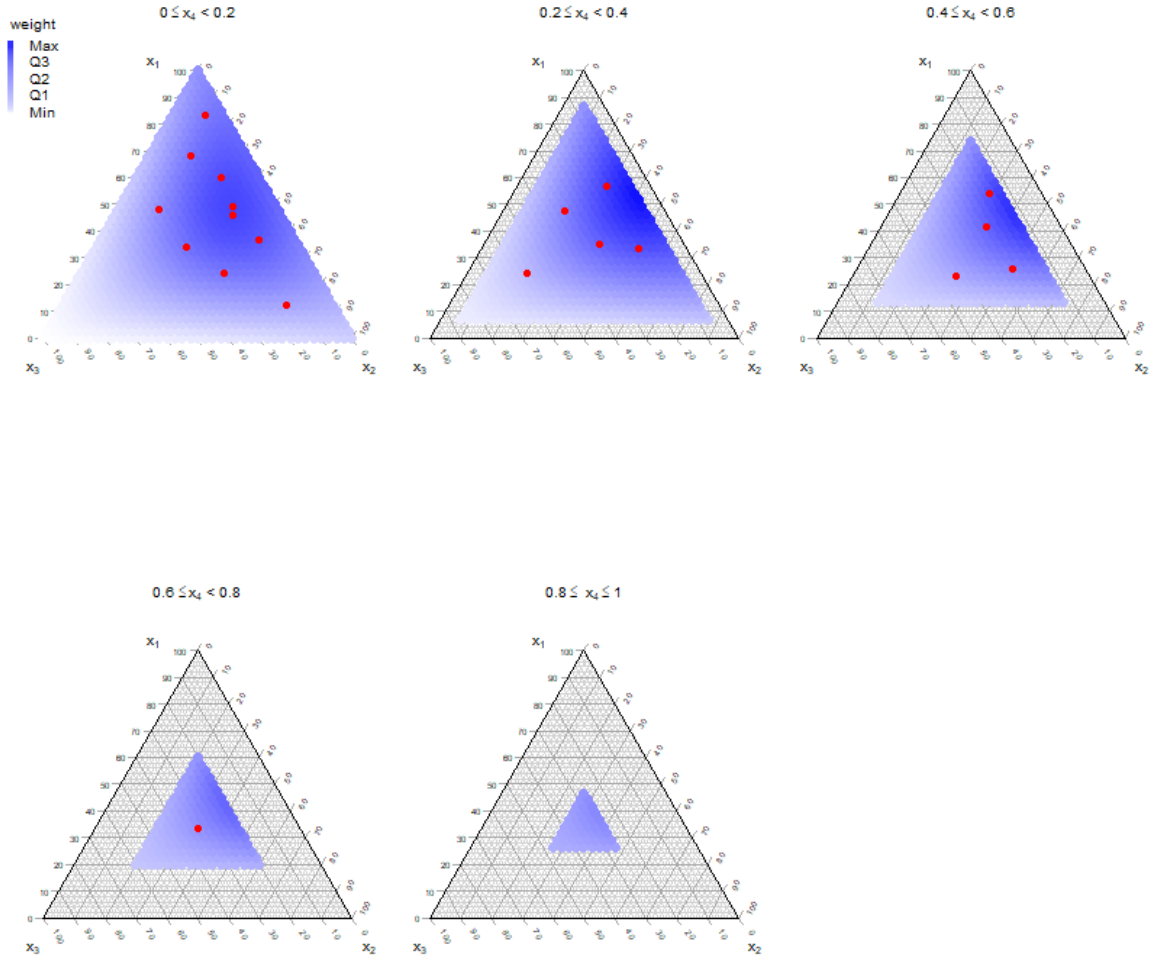


- For 3D mixture data, we use a shaded contour ternary plot to summarize the weight distribution of candidate points. The darker blue shades correspond to regions with higher weights, and the lighter blue corresponds to lower weights. The red points in right plot represent the design points selected for the constructed design.



- For 4D mixture data, we show slices at selected values of one of the input factors from a shaded contour ternary plot to summarize the weight distribution from the candidate set (Lu & Anderson-Cook, 2014). x_4 represents the orthogonal distance of a point from the face where $x_4 = 0$. Each ternary plot for a specific range of x_4 shows a color contour of x_4 with the low value of the range.

Darker blue shades indicate regions with higher weights, while lighter blue shades correspond to regions with lower weights. Red points represent the design points selected for the constructed design. These red points, shown in each sliced plot, indicate the projected design points located within the corresponding range of x_4, as indicated in the title of each sliced ternary plot, even though they are not exactly on the cross-section at the smallest x_4 value shown as the inner triangle in blue shades.



References

Lu, L., & Anderson-Cook, C. M. (2014). Balancing multiple criteria incorporating cost using Pareto front optimization for split-plot designed experiments. *Quality and Reliability Engineering International*, *30*(1), 37-55.