Stable Isotope Sourcing using Sampling
Getting Started

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S_{table} I_{sotope} $S_{ourcing}$ U_{sing} $S_{ampling}$

http://StatAcumen.com/sisus

Contents

I sincerely hope you enjoy using SISUS and you find it adds value to your understanding of the systems you study. I appreciate comments and suggestions by email.

Regards,
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Stable Isotope Sourcing Using Sampling

1   Overview

Stable Isotope Sourcing using Sampling is an approximate Bayes statistical procedure and software solving stable isotope sourcing diet mixing models including discrimination (fractionation), concentration, and assimilation efficiency. SISUS uses a single Excel workbook as an input file to run in R. The workbook has been tested using OpenOffice.org, an open source, freely available office suite that runs on all popular operating systems, including Mac OSX and Linux. The Excel worksheets specify the execution parameters, data, and assumptions for the analysis or the information to replace those assumptions. This design has the advantage of keeping all running parameters and data in one place, and simplifies the input interface. The ability to include information such as source elemental concentration, assimilation efficiency, additional linear constraints and prior expert knowledge allows accurate inferences to be made. Switches on the Parameters worksheet allows the user to toggle between using a simpler model with assumptions or to include the data in each sheet in the model in place of the assumptions.

2   Installing software

Installation is only required once.

2.1   Supporting software

R and Perl are required. RStudio may make your experience more enjoyable.
1. R (sisus requires R 3.0.0+)
    - Windows `http://cran.r-project.org/bin/windows/base/` or
    - Mac `http://cran.r-project.org/bin/macosx/`
2. RStudio
    - RStudio `http://www.rstudio.org/download/` nicer GUI
3. Perl
    - Mac and linux, you already have it installed
    - Windows
        - Install `http://www.activestate.com/activeperl/downloads`
        - Change the path variable to include `C:\Perl\bin` (location on your machine): `http://www.java.com/en/download/help/path.xml`

2.2   SISUS software

Run R (or RStudio) and at the R prompt type `install.packages("sisus")` to install SISUS.

If that doesn't work, download the current `sisus_3.9-14.tar.gz` (version number may differ) from `cran.r-project.org/package=sisus`, set the working directory to where you downloaded the file (such as `setwd("C:/path/to/file/")`) and run the same command with options:
`install.packages("sisus_3.9-14.tar.gz", type="source", repos = NULL)`

3   Using SISUS

Provided you have data ready to analyze, there are a few simple steps to getting quick, accurate, and attractive results using SISUS.

1. Copy the template file to a new directory or folder on your computer for this analysis.
   - File is located in your sisus installation, for example at
     `C:\Program Files\R\R-3.1.2\library\sisus\extdata\SISUS_v0_09_template.xls`.
   - Alternatively, visit http://StatAcumen.com/sisus and download the Workbook.
2. Input your data in the Workbook, setting the parameter values that correspond to your desired analysis. See Workbook details below.
3. Run sisus using the Workbook as an input file.
   - `library(sisus)`
   - `path <-"C:/path/to/your/workbook"`
   - `setwd(path)`
   - `filename <-"SISUS_MyData.xls"`
   - `sisus.run(filename)`
4. Results are written to the directory or folder with your Workbook.

3.1   Workbook

The workbook has been designed to allow maximum clarity and flexibility of use. In this section, I describe each of the included worksheets, and cover each part of each worksheet in detail.

I have protected the sheets of the workbook so that only valid input is allowed in each field. The sheets can be easily unprotected (Menu: Tools/Protection/Unprotect Sheet), and you could turn validation off, though you invite errors in execution if bad values are entered.

3.1.1 Worksheet 1, SISUS Parameters

Worksheet 1 is where execution parameters are set and will be described in detail in the following subsections describing each heading of the Parameters worksheet.

	A	B	C	D
1	**SISUS Parameters**	**Settings**	*Values*	**Description**
2	**Analysis Labels**	*SISUS v0.08*		
3	analysis.name	SISUS Getting Started	*long text*	name of this analysis to print on plots and tables
4	filename.prefix	SISUS_GS_v0_08	*short string*	character string (no spaces) at beginning of all output filenames (if blank, default is "SISUS")
5	mixtures.group.name	Mixtures Group Name	*short string*	If n.mixtures > 1, then name the group of mixtures
6	**Data Dimensions**			
7	n.mixtures	3	*1 or more*	number of mixtures to analyze together
8	n.sources	4	*2 or more*	n = number of sources composing the mixture
9	n.isotopes	2	*1 or more*	k = number of isotopes measured
10	**Sampling**			
11	M	10000	*10000 or so*	total number of samples to retain
12	skip	100	*100 or so*	draw [skip] samples from the polytope keeping the last one
13	burnin	10	*10 or so*	number of samples to draw to get off the boundary of the polytope (there is a check to guarent...
14	seed	76543	*0-100000*	random seed (to repeat results)
15	**Mixing Model**			
16	simplex.include.sw	1	*(1=use, 0=ignore)*	Include simplex constraint (1=yes, usually estimating proportion of diet; 0=no, estimating fract...
17	discrimination.include.sw	1	*(1=use, 0=ignore)*	Correct for discrimination using values on Discrimination worksheet (Source Isotopic Values + ...
18	concentration.include.sw	1	*(1=use, 0=ignore)*	Include concentration dependence
19	assimeffic.include.sw	0	*(1=use, 0=ignore)*	Include assimilation efficiency
20	lc.include.sw	1	*(1=use, 0=ignore)*	Use defined Linear Constraints
21	prior.include.sw	1	*(1=use, 0=ignore)*	Resample uniform sampe based on defined Dirichlet distribution
22	isotope.stddev.include.sw	1	*(1=use, 0=ignore)*	Isotope standard deviations used for error bars on convex hull plots
23	biomass.per.individual.include.sw	0	*(1=use, 0=ignore)*	Use Biomass per Individual and Number of Individuals in Proportions of Source Consumed mo...
24	**Output Settings**			
25	plot.convex.hull.include.sw	1	*(1=make ,0=don't)*	Output Convex Hull plot
26	plot.marginal.histogram.include.sw	1	*(1=make ,0=don't)*	Output Marginal Histogram plot
27	plot.scatterplot.matrix.include.sw	1	*(1=make ,0=don't)*	Output Scatterplot Matrix
28	numerical.summaries.include.sw	1	*(1=make ,0=don't)*	Output Numerical Summaries and Statistics
29	solution.polytope.vertices.sw	1	*(1=make ,0=don't)*	Output solution polytope verticies as part of numerical summary
30	samples.include.sw	1	*(1=make ,0=don't)*	Output solution polytope samples
31	time.series.sw	0	*(1=make ,0=don't)*	Output list of means for multiple mixtures as a series over time
32	hist.bins	10	10	number of bins for histograms in marginal histogram plots
33	hist.density.sw	1	*(1=use, 0=ignore)*	Overlay a density smoother on the marginal histogram plots
34	**Plot Formats**			
35	plot.type.png	1	*(1=make ,0=don't)*	produce plots in (.png) Portable Network Graphics format (0=no, 1=yes) (lossless for web) (Al...
36	plot.type.eps	1	*(1=make ,0=don't)*	produce plots in (.eps) Encapsulated PostScript format (0=no, 1=yes) (for LaTeX and *nix)
37	plot.type.pdf	0	*(1=make ,0=don't)*	produce plots in (.pdf) Portable Document Format format (0=no, 1=yes) (for pdfLaTeX)
38	plot.type.bmp	0	*(1=make ,0=don't)*	produce plots in (.bmp) Windows and OS/2 bitmap format (0=no, 1=yes) (for Windows)
39	plot.type.jpeg	0	*(1=make ,0=don't)*	produce plots in (.jpeg) Joint Photographic Experts Group format (0=no, 1=yes) (compressed ...
40	plot.type.gif	0	*(1=make ,0=don't)*	produce plots in (.gif) Graphics Interchange Format (0=no, 1=yes) (compressed)
41				
42			*Color Key:*	**Worksheet Titles**
43				Unchangable Cells
44				Changeable Cells, for "no effect" or "default"
45				Changeable Cells, for "effect" or "setting"
46				"Proportions of Sources Consumed Mixing Model" does not use Simplex

Figure 1: Worksheet 1, SISUS Parameters

3.1.2   Worksheet 1, SISUS Parameters: Analysis Labels

The Analysis Labels section defines three variables used for labelling output and filenames.

analysis.name Appears in plots and numerical summaries as a subtitle.

filename.prefix A common prefix to all output files from SISUS. If you save all your files in the same directory (folder) on your computer, than this is a way to distinguish them.

mixtures.group.name If you specify more than one mixture, then this is the label that is used to specify the group of mixtures. This appears on group Convex Hull plots.

	A	B	C
1	**SISUS Parameters**	**Settings**	*Values*
2	**Analysis Labels**	*SISUS v0.08*	
3	analysis.name	SISUS Getting Started	*long text*
4	filename.prefix	SISUS_GS_v0_08	*short string*
5	mixtures.group.name	Mixtures Group Name	*short string*

Figure 2: Worksheet 1, SISUS Parameters: Analysis Labels

3.1.3   Worksheet 1, SISUS Parameters: Data Dimensions

The Data Dimensions section specifies the number of mixtures, sources and isotopes. If you have more than the numbers specified here, it uses only the number specified. If you specify more than you have in the worksheets, then you may experience an error.

n.mixtures Number of mixtures specified in worksheet 2.

n.sources Number of sources specified in worksheet 3.

n.isotopes Number of isotopes specified in worksheet 2.

6	**Data Dimensions**		
7	n.mixtures	3	1 or more
8	n.sources	4	2 or more
9	n.isotopes	2	1 or more

Figure 3: Worksheet 1, SISUS Parameters: Data Dimensions

3.1.4 Worksheet 1, SISUS Parameters: Sampling

The Sampling section specifies how the samples are collected.

M Total number of samples to retain for analysis.

skip During MCMC sampling procedure, a skip value of 100 indicates that every 100th sample will be retained for analysis, to improve coverage of the solution space and reduce autocorrelation.

burnin Number of samples before retaining for analysis.

seed Seed to initialize the random number generator. Running with the same seed will give the same results. Changing the seed will provide a different sample, yet with enough samples, the results will be comparable. The spreadsheet has this defined to be a different random number each time the file is changed or saved, so replace with an integer for repeatability.

10	**Sampling**		
11	M	10000	*10000 or so*
12	skip	100	*100 or so*
13	burnin	10	*10 or so*
14	seed	76543	*0-100000*

Figure 4: Worksheet 1, SISUS Parameters: Sampling

3.1.5   Worksheet 1, SISUS Parameters: Mixing Model

The Mixing Model section specifies the information you want included as part of the mixing model. Most of these switches indicate you want to replace an assumption of a simpler model by values specified in one of the worksheets for a better informed model.

simplex.include.sw Include the constraint that the sum of the proportions is 1; this constraint is called the "simplex".

discrimination.include.sw Use spreadsheet 4, correct source isotope ratios by add the discrimination values.

concentration.include.sw Use spreadsheet 5, incorporate concentration dependence in the model.

assimeffic.include.sw Use spreadsheet 6, incorporate assimilation efficiency dependence in the model.

lc.include.sw Use spreadsheet 7, use the linear constraints to further restrict the solutions.

prior.include.sw Use spreadsheet 8, resample based on prior information (expert opinion).

isotope.stddev.include.sw Use spreadsheets 9 and 10, display error bars on Convex Hull plots (not used in calculations).

biomass.per.individual.include.sw Use spreadsheet 11, use population biomass in proportions of sources consumed mixing model, also need to turn off `simplex.include.sw`.

15	**Mixing Model**		
16	simplex.include.sw	1	(1=use, 0=ignore)
17	discrimination.include.sw	1	(1=use, 0=ignore)
18	concentration.include.sw	1	(1=use, 0=ignore)
19	assimeffic.include.sw	0	(1=use, 0=ignore)
20	lc.include.sw	1	(1=use, 0=ignore)
21	prior.include.sw	1	(1=use, 0=ignore)
22	isotope.stddev.include.sw	1	(1=use, 0=ignore)
23	biomass.per.individual.include.sw	0	(1=use, 0=ignore)

Figure 5: Worksheet 1, SISUS Parameters: Mixing Model

3.1.6   Worksheet 1, SISUS Parameters: Output Settings

The Output Settings section specifies the way some of the output appears.

plot.convex.hull.include.sw   Output Convex Hull plot

plot.marginal.histogram.include.sw Output Marginal Histogram plot

plot.scatterplot.matrix.include.sw Output Scatterplot Matrix (takes a long time for large sample size M)

numerical.summaries.include.sw   Output Numerical Summaries and Statistics

solution.polytope.vertices.sw   Output solution polytope verticies as part of numerical summary

samples.include.sw   Output solution polytope samples

time.series.sw   Output list of means (or unique solutions) for multiple mixtures as a series over time. For when long list of mixtures are taken over time to plot over time.

hist.bins   The number of bins used in the marginal histograms.

hist.density.sw   Overlay a density smoother on the marginal histogram plots

24	Output Settings		
25	plot.convex.hull.include.sw	1	(1=make ,0=don't)
26	plot.marginal.histogram.include.sw	1	(1=make ,0=don't)
27	plot.scatterplot.matrix.include.sw	1	(1=make ,0=don't)
28	numerical.summaries.include.sw	1	(1=make ,0=don't)
29	solution.polytope.vertices.sw	1	(1=make ,0=don't)
30	samples.include.sw	1	(1=make ,0=don't)
31	time.series.sw	0	(1=make ,0=don't)
32	hist.bins	10	10
33	hist.density.sw	1	(1=use, 0=ignore)

Figure 6: Worksheet 1, SISUS Parameters: Output Settings

3.1.7   Worksheet 1, SISUS Parameters: Plot Formats

The Plot Formats section specifies which file format the plots will be created in. Multiple formats can be selected. For example, LATEX users might output vector formats eps and pdf (for LATEX and pdfLATEX), while users of MS Word might prefer raster formats bmp, jpeg, or gif. The png format is nice for websites, and outputs automatically because it is quick to view on the results page and is used to convert to the other raster formats.

plot.type.png (.png) Portable Network Graphics format

plot.type.eps (.eps) Encapsulated PostScript format

plot.type.pdf (.pdf) Portable Document Format format

plot.type.bmp (.bmp) Windows and OS/2 bitmap format

plot.type.jpeg (.jpeg) Joint Photographic Experts Group format

plot.type.gif (.gif) Graphics Interchange Format

34	**Plot Formats**		
35	plot.type.png	1	(1=make ,0=don't)
36	plot.type.eps	0	(1=make ,0=don't)
37	plot.type.pdf	0	(1=make ,0=don't)
38	plot.type.bmp	0	(1=make ,0=don't)
39	plot.type.jpeg	0	(1=make ,0=don't)
40	plot.type.gif	0	(1=make ,0=don't)

Figure 7: Worksheet 1, SISUS Parameters: Plot Formats

3.1.8 Worksheet 1, SISUS Parameters: Color Key

The Workbook has color-coded fields to clarify the settings.

Orange Used for titles of worksheets.

Green Cells that are information only, not used as SISUS input.

Blue Cells that specify input

Light Blue Used for default settings, or settings that have no effect.

Dark Blue Used for settings that have an effect.

Purple If the simplex condition is removed, the interpretation of the mixing model changes to "Fraction of Sources Consumed by Mixture" and Sources Concentrations should be specified as total Biomass of each source in consumable environment.
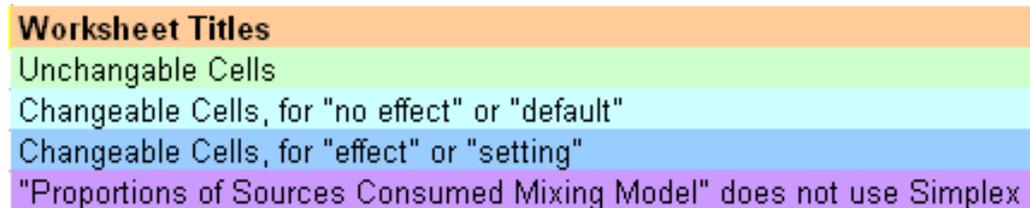
Figure 8: Worksheet 1, SISUS Parameters: Color Key

3.1.9   Worksheet 2, Mixtures Isotope Ratios

Worksheet 2 defines three items.

Isotope Names Isotopes are defined as columns, and the Isotope names are specified as the column headers.

Mixture Names Mixtures are defined as rows, and the Mixture names are specified as the row labels.

Mixture Isotope Ratios The isotope ratios observed in each mixture, $\delta E_{M,j}$ for $i = 1, \ldots, k$ isotopes.

The names of the mixtures and isotopes on this sheet are referenced on subsequent spreadsheets. Data Dimensions parameters `n.mixtures` and `n.isotopes` in Worksheet 1 should be set to the number mixtures and isotopes defined.

	A	B	C	D	E	F
1	**Mixtures Isotopic Values**	Isotope 1	Isotope 2			
2	Mixture 1	0.00	0.00			
3	Mixture 2	0.50	0.50			
4	Mixture 3	-0.50	-0.25			
5						
6						
7						
8						
9						
10						

Figure 9: Worksheet 2, Mixtures Isotope Ratios

3.1.10 Worksheet 3, Sources Isotope Ratios

Worksheet 3 defines two items. Notice that the Isotope names are copied from Worksheet 2.

Source Names Sources are defined as rows, and the Source names are specified as the row labels.

Source Isotope Ratios The isotope ratios observed in each source, $\delta E_{i,j}$ for $s = 1, \ldots, n$ sources and $i = 1, \ldots, k$ isotopes.

The names of the sources on this sheet are referenced on subsequent spreadsheets. Data Dimensions parameters `n.sources` in Worksheet 1 should be set to the number sources defined.

	A	B	C	D	E	F
1	**Sources Isotopic Values**	Isotope 1	Isotope 2	0	0	0
2	Source 1	0.25	-1.00			
3	Source 2	-0.25	1.00			
4	Source 3	-1.00	-0.25			
5	Source 4	1.00	0.25			
6						
7						
8						
9						
10						

Figure 10: Worksheet 3, Sources Isotope Ratios

3.1.11　Worksheet 4, Sources Discrimination

Worksheet 4 defines discrimination values $\Delta E_{i,j}$ and is used only if Mixing Model parameter `discrimination.include.sw` is turned on (set to 1) in Worksheet 1. The ultimate source isotope values used in the model are $\delta E_{i',j} = \delta E_{i,j} + \Delta E_{i,j}$.

	A	B	C	D	E	F
1	**Sources Discrimination**	Isotope 1	Isotope 2	0	0	0
2	Source 1	0.00	0.00	0.00	0.00	0.00
3	Source 2	0.00	0.00	0.00	0.00	0.00
4	Source 3	0.00	0.00	0.00	0.00	0.00
5	Source 4	0.00	0.00	0.00	0.00	0.00
6	0	0.00	0.00	0.00	0.00	0.00
7	0	0.00	0.00	0.00	0.00	0.00
8	0	0.00	0.00	0.00	0.00	0.00
9	0	0.00	0.00	0.00	0.00	0.00
10	0	0.00	0.00	0.00	0.00	0.00

Figure 11: Worksheet 4, Sources Discrimination

3.1.12 Worksheet 5, Sources Concentration

Worksheet 5 defines source concentration values $[E_{i,j}]$, the relative concentration of each element in the sources, as in the concentration mixing model, and is used only if Mixing Model parameter `concentration.include.sw` is turned on (set to 1) in Worksheet 1. These values are relative by element in that if a column is scaled, the results are the same.

	A	B	C	D	E	F
1	**Sources Concentration**	Isotope 1	Isotope 2	0	0	0
2	Source 1	2.00	1.00	1.00	1.00	1.00
3	Source 2	10.00	5.00	1.00	1.00	1.00
4	Source 3	2.00	2.00	1.00	1.00	1.00
5	Source 4	1.00	2.00	1.00	1.00	1.00
6	0	1.00	1.00	1.00	1.00	1.00
7	0	1.00	1.00	1.00	1.00	1.00
8	0	1.00	1.00	1.00	1.00	1.00
9	0	1.00	1.00	1.00	1.00	1.00
10	0	1.00	1.00	1.00	1.00	1.00

Figure 12: Worksheet 5, Sources Concentration

3.1.13 Worksheet 6, Sources Assimilation Efficiency

Worksheet 6 defines source assimilation efficiency values $e_{i,j}$, the relative efficiency of each element in the sources to be incorporated into the mixture, as in the extended mixing model, and is used only if Mixing Model parameter `assimeffic.include.sw` is turned on (set to 1) in Worksheet 1. These values are relative by element in that if a column is scaled, the results are the same.

	A	B	C	D	E	F
1	**Sources Assimilation Efficiency**	Isotope 1	Isotope 2	0	0	0
2	Source 1	1.00	1.00	1.00	1.00	1.00
3	Source 2	1.00	1.00	1.00	1.00	1.00
4	Source 3	1.00	1.00	1.00	1.00	1.00
5	Source 4	1.00	1.00	1.00	1.00	1.00
6	0	1.00	1.00	1.00	1.00	1.00
7	0	1.00	1.00	1.00	1.00	1.00
8	0	1.00	1.00	1.00	1.00	1.00
9	0	1.00	1.00	1.00	1.00	1.00
10	0	1.00	1.00	1.00	1.00	1.00

Figure 13: Worksheet 6, Sources Assimilation Efficiency

3.1.14   Worksheet 7, Linear Constraints

Worksheet 7 defines additional linear constraints, and because of the flexibility will be described in some detail. SISUS has been designed to accommodate any number of arbitrary linear constraints. There are three columns to set the source contributions Equal to specified proportions, or to set the Minimum or Maximum contributions of sources. Any number of additional columns may be added for linear constraints consisting of more than one source. Add a column, label it EQ, LE, or GE for equal, less than or equal, or greater than or equal, respectively, and define the coefficients of the constraint. For example, assume we have four sources to specify and we want to specify that the contribution of source 3 should be twice that of source 2. Use the equation $1p_1 + 2p_2 + \cdots + np_S = b$, where $\{1, 2, \ldots, n\}$ are values set in the source rows used to create a linear equality to "$= b$" set in the RHS b row. The desired EQ column specifies the equation $0p_1 + 2p_2 - 1p_3 + 0p_4 = 0$, or $2p_2 - 1p_3 = 0$, or $p_3 = 2p_2$. The coefficients for this example are in Table 1 on page 19 below. The same is true for LE and GE, but the equation has "$\leq b$" and "$\geq b$", respectively.

Table 1: Worksheet 7, Linear Constraints: Example where proportion contribution of source 3 is exactly twice that of source 2.

Linear Constraints	Equal	Minimum	Maximum	EQ
RHS b				0
Source 1				0
Source 2				2
Source 3				−1
Source 4				0

Figure 14: Worksheet 7, Linear Constraints: Showing Source 4 ≥ Source 2

3.1.15   Worksheet 8, Prior

Worksheet 8 is used for incorporating prior information (expert opinion) on source proportion vector p_B. The values specified in the spreadsheet defines a Dirichlet distribution on the simplex used in the sampling-importance re-sampling (SIR) procedure; the simplex is the constraint that the sum of the source proportions is 1. The values a_i and precision π define Dirichlet parameters $\alpha_s = \pi a_i$; for example, a uniform distribution is given as $a_s = \frac{1}{S}$ and precision is n, so that $\alpha_s = 1, s = 1, \ldots, n$. The default is that every point in the simplex has equal probability of being sampled, that is, all combinations of proportions that sum to 1 are equally likely. If we have information that the mixture is likely to use more of some sources than others, then before seeing the data, *a priori*, we can specify that information here. We define a Dirichlet prior distribution on the simplex used in a sampling-importance resampling (SIR) procedure.

Procedure: We first define the mean (average) proportion vector p, this is what we believe the source contributions to the mixture are. Then we define a precision, this is how strongly we believe this (the inverse of "variation"). For example, the uniform distribution has equal proportions that sum to 1 for the sources and a precision of 1; larger precisions will have a stronger tendency to group tightly around the specified mean. After the uniform samples are drawn, these samples are reweighted by the Dirichlet distribution and a weighted resampling is performed. Both the original samples and these resamples are summarized for both results and to compare to understand what effect the prior had on the inference. In the process_info.txt output, information is given regarding the Dirichlet prior specified.

	A	B	C	D	E	F
1	**Priors**	p proportions				
2	Precision	1.00				
3	Source 1	0.20				
4	Source 2	0.10				
5	Source 3	0.20				
6	Source 4	0.50				
7	0					
8	0					
9	0					
10	0					

Figure 15: Worksheet 8, Priors

3.1.16   Worksheet 9, Mixtures Isotope StdDev

Worksheet 9 defines the estimated population standard deviation of the Mixtures isotope ratios. Currently, this variation is not used in calculations, but will appear on the convex hull plots.

	A	B	C	D	E	F
1	**Mixtures Isotope StdDev**	Isotope 1	Isotope 2	0	0	0
2	Mixture 1	0.20	0.30	0.00	0.00	0.00
3	Mixture 2	0.00	0.00	0.00	0.00	0.00
4	Mixture 3	0.00	0.00	0.00	0.00	0.00
5	0	0.00	0.00	0.00	0.00	0.00
6	0	0.00	0.00	0.00	0.00	0.00
7	0	0.00	0.00	0.00	0.00	0.00
8	0	0.00	0.00	0.00	0.00	0.00
9	0	0.00	0.00	0.00	0.00	0.00
10	0	0.00	0.00	0.00	0.00	0.00

Figure 16: Worksheet 9, Mixtures Isotope StdDev

3.1.17 Worksheet 10, Sources Isotope StdDev

Worksheet 10 defines the estimated population standard deviation of the Sources isotope ratios. Currently, this variation is not used in calculations, but will appear on the convex hull plots.

	A	B	C	D	E	F
1	**Sources Isotope StdDev**	Isotope 1	Isotope 2	0	0	0
2	Source 1	0.10	0.20	0.00	0.00	0.00
3	Source 2	0.00	0.00	0.00	0.00	0.00
4	Source 3	0.50	0.40	0.00	0.00	0.00
5	Source 4	0.00	0.00	0.00	0.00	0.00
6	0	0.00	0.00	0.00	0.00	0.00
7	0	0.00	0.00	0.00	0.00	0.00
8	0	0.00	0.00	0.00	0.00	0.00
9	0	0.00	0.00	0.00	0.00	0.00
10	0	0.00	0.00	0.00	0.00	0.00

Figure 17: Worksheet 10, Sources Isotope StdDev

3.1.18   Worksheet 11, Sources Biomass per Individual

Worksheet 11 defines the consumable biomasses of sources, as in the proportions of sources consumed mixing model. Let B_i be the consumable biomass of source i, conveniently computed as the product of BPI_i, the biomass per individual for source i (first column), and NCI_i, the number of consumable individuals for source i (second column), $B_s = BPI_i \times NCI_i$.

	A	B	C	D	E	F
1	**Sources Biomass per Individual**	Biomass	Number			
2	Source 1	1.00	1.00			
3	Source 2	1.00	1.00			
4	Source 3	1.00	1.00			
5	Source 4	1.00	1.00			
6	0	1.00	1.00			
7	0	1.00	1.00			
8	0	1.00	1.00			
9	0	1.00	1.00			
10	0	1.00	1.00			

Figure 18: Worksheet 11, Sources Biomass per Individual

3.2   Results

The results are a list of files. The output requested in Output Settings of Worksheet 1 are written out. All the output files have the specified [filename.prefix] as the initial string in the filename. File suffixes may include the mixture name and isotope names. In the filenames given below, only the core distinguishing name is given. The results files are grouped in this order.

1. Workbook, submitted file

2. [filename.prefix]_process_info.txt, copy of the Process Log window. **This file should be the first file reviewed to see whether there were solutions to the system, and reviewed for settings actually used in analysis as well as resulting model assumptions.**

3. sisus_inputs.txt, a text version of the worksheets used from the submitted Workbook — a quick way to check the settings if the workbook isn't available.

4. Convex Hull plots, first for each mixture alone, then the mixture group if more than one mixture.

   (a) For each mixture, Convex Hull plots for each elemental pair is given, then a matrix plot of all pairs together.

5. For each mixture for which solutions exist there is a set of files

   (a) plot_marginal_hist_unif_sam, Marginal histogram of feasible source proportions for uniform sampling.

   (b) If prior specified, plot_marginal_hist_Dir_resam, Marginal histogram of feasible source proportions for Dirichlet resampling.

   (c) sisus_stats.txt, numerical summaries

   (d) sisus_samples.csv, the samples used for plots and numerical summaries

   (e) If prior specified, sisus_resamples.csv, the resamples used for plots and numerical summaries

   (f) plot_scatterplot_matrix, Scatterplot matrix of proportions for all pairs of sources.

6. For all mixtures together, sisus_stats_timeseries_ txt and csv files with list of means (or unique solutions) for multiple mixtures as a series over time.

3.2.1   Process Log

This file should be checked first for the status of the execution. Figures 19–20 on pages 27–28 shows the process log for the submitted template. The "... [seconds]" indicates a progress line, the number of seconds ellapsed since starting program execution, and a note about what process step has begun.

Reading workbook specifies the workbook file, and places an "r" after each workbook read specified by the switches in worksheet 1.

SISUS Model Settings gives some of the settings defined on worksheet 1 to confirm the intentions of the user.

SISUS Model Assumptions specifies the assumptions made by either including or failing to include information in later worksheets in the workbook. The more information included, the fewer model assumptions are being made.

SISUS Output Settings specifies the settings that determine the output created.

Set random seed recovers the seed used if results are to be repeated.

Dirichlet prior on p vector Specifies information about the prior, if one was specified.

Plot Augmented Convex Hull First create convex hull plots.

For each Mixture computations are done seperately

   process Mixture: mixture name Indicates mixture being processed.

   Draw uniform samples Tells the number of vertices in the solution polytope.

   Number of samples leading to feasible solutions   If no solutions exist a warning is given here, and no output files are generated for the mixture.
   `Information:  No feasible solutions.  Check Convex Hull plots.`

   Resample based on specified prior.

   Back-solve from Biomass solutions to elemental contribution.

   Plots and Numerical Output Mixture specific output section

      Uniform Sample Original uniform samples from solution polytope
         For Biomass, then for each isotope (if concentrations or assimilation efficiencies are specified)
         Marginal Histograms quick

       Scatterplot Matrix slow

       Numerical Summaries quick

   Write out samples csv file

   Dirichlet Resample Resample uniform samples weighted by Dirichlet prior on simplex

       For Biomass, then for each isotope (if concentrations or assimilation efficiencies are specified)

       Marginal Histograms quick

       Scatterplot Matrix slow

       Numerical Summaries quick

   Write out samples csv file

SISUS Complete and total time in seconds for execution.

```
>     0.00 SISUS: Stable Isotope Sourcing using Sampling
          http://StatAcumen.com/sisus, by Erik Barry Erhardt
          Starting  Tue May 29 21:48:48 2007   Version:  v.0.08-010
>     0.01 Reading workbook:  SISUS_v0_08-010_Getting_Started.xls
      reading up to  11 sheets, as requested:   1r  2r  3r  4r  5r  6  7r  8r  9r  10r  11
>    24.08 Process input data and assign variables

### SISUS Model Settings ###
  analysis.name =  SISUS Getting Started
  filename.prefix =  SISUS_GS_v0_08
  mixtures.group.name =  Mixtures Group Name

  m =  3  Mixtures
  n =  4  Sources
  k =  2  Isotopes

  Include SIMPLEX (sum of proportions is 1) constraint -- for Mixing Model

  Correcting source isotope ratios for discrimination
  Using SOURCE CONCENTRATIONS
  NOT using ASSIMILATION EFFICIENCIES
  Including additional LINEAR CONSTRAINTS
  Importance resampling using PRIOR weighting of uniform samples, if specified, in addition to uniform samples from sol
  Including ISOTOPE STDDEV on Convex Hull plots
  NOT using BIOMASS PER INDIVIDUAL
  NOT using NUMBER OF INDIVIDUALS

### SISUS Model Assumptions (under development) ###
  Mixing Model using Simplex
  Discrimination values are accurately specified.
  Elemental concentrations are accurately specified.
  Assimilation efficiencies are the same for all sources and elements.
  Additional linear constraints are accurately specified.
  Prior (expert) knowledge properly specified as Dirichlet distribution over the simplex.
  NOT using BIOMASS PER INDIVIDUAL
  NOT using NUMBER OF INDIVIDUALS

### SISUS Output Settings ###

  Mixtures are not a time series

>    24.24 Set random seed = 76543
>    24.25 Dirichlet prior on p vector
            Dirichlet prior on p vector
            Input priors:     0.2, 0.1, 0.2, 0.5
            Input precision:  1
            Alphas:    0.8, 0.4, 0.8, 2
            Expected:  0.2, 0.1, 0.2, 0.5
            Variance:  0.032, 0.018, 0.032, 0.05
            StdDev:    0.178885438199983, 0.134164078649987, 0.178885438199983, 0.223606797749979
>    24.26 Dirichlet prior for p is not uniform -- resample
>    24.26 Draw 0 samples from MVN isotope distribution
>    24.36 Plot Convex Hull

==> process Mixture:  Mixture 1
>    33.66 Draw uniform samples from convex solution polytope
            Drawing 1 sample(s) of size 10000 for a total of  10000 samples:
            1  (v)
            Solution Polytope with 2 vertices
>    63.43 1  of  1  =  100 % of mvn samples lead to feasible solutions
>    63.43 Resample based on Dirichlet prior for p, with parameters alpha= 0.8 0.4 0.8 2
>    70.00 Back-solve from biomass to isotopes contributions
>    90.27 Plots and Numerical Output
>    90.28    Uniform Sample
>    90.28       Biomass Marginal Histogram
>    91.42       Biomass Scatterplot Matrix (long time for large samples)
>   135.06       Biomass Numerical Summaries
```

Figure 19: Results, devel_v01-07_process_info.txt (1 of 2)

```
>  135.30        Isotope 1 Marginal Histogram
>  136.25        Isotope 1 Scatterplot Matrix (long time for large samples)
>  177.23        Isotope 1 Numerical Summaries
>  177.33        Isotope 2 Marginal Histogram
>  178.19        Isotope 2 Scatterplot Matrix (long time for large samples)
>  218.28        Isotope 2 Numerical Summaries
>  218.38     Write out samples
>  219.04     Dirichlet Resample
>  219.05        Biomass Marginal Histogram
>  219.76        Biomass Scatterplot Matrix (long time for large samples)
>  271.22        Biomass Numerical Summaries
>  271.36        Isotope 1 Marginal Histogram
>  272.01        Isotope 1 Scatterplot Matrix (long time for large samples)
>  314.61        Isotope 1 Numerical Summaries
>  314.71        Isotope 2 Marginal Histogram
>  315.36        Isotope 2 Scatterplot Matrix (long time for large samples)
>  361.46        Isotope 2 Numerical Summaries
>  361.56     Write out samples

==> process Mixture:  Mixture 2
>  362.25 Draw uniform samples from convex solution polytope
          Drawing 1 sample(s) of size 10000 for a total of  10000 samples:
          1  (v)
          WARNING: No vertices in solution polytope, Unfeasible Solution -- check Convex Hull plots.

          Solution Polytope with 0 vertices
>  362.27 0  of  1  =  0 % of mvn samples lead to feasible solutions

Information:  No feasible solutions.  Check Convex Hull plots.


==> process Mixture:  Mixture 3
>  362.28 Draw uniform samples from convex solution polytope
          Drawing 1 sample(s) of size 10000 for a total of  10000 samples:
          1  (v)
          Solution Polytope with 2 vertices
>  392.95 1  of  1  =  100 % of mvn samples lead to feasible solutions
>  392.95 Resample based on Dirichlet prior for p, with parameters alpha= 0.8 0.4 0.8 2
>  400.23 Back-solve from biomass to isotopes contributions
>  420.77 Plots and Numerical Output
>  420.77    Uniform Sample
>  420.77        Biomass Marginal Histogram
>  421.50        Biomass Scatterplot Matrix (long time for large samples)
>  471.74        Biomass Numerical Summaries
>  471.88        Isotope 1 Marginal Histogram
>  472.54        Isotope 1 Scatterplot Matrix (long time for large samples)
>  512.87        Isotope 1 Numerical Summaries
>  512.96        Isotope 2 Marginal Histogram
>  513.88        Isotope 2 Scatterplot Matrix (long time for large samples)
>  556.70        Isotope 2 Numerical Summaries
>  557.01     Write out samples
>  557.70     Dirichlet Resample
>  557.70        Biomass Marginal Histogram
>  558.40        Biomass Scatterplot Matrix (long time for large samples)
>  603.40        Biomass Numerical Summaries
>  603.54        Isotope 1 Marginal Histogram
>  604.17        Isotope 1 Scatterplot Matrix (long time for large samples)
>  648.08        Isotope 1 Numerical Summaries
>  648.18        Isotope 2 Marginal Histogram
>  648.80        Isotope 2 Scatterplot Matrix (long time for large samples)
>  689.75        Isotope 2 Numerical Summaries
>  689.84     Write out samples

>  690.52 SISUS Complete
```

Figure 20: Results, devel_v01-07_process_info.txt (2 of 2)

3.2.2   Plots

All plots have four common properties. At the bottom, credit is given to Stable Isotope Sourcing using Sampling. On the left, the number of sources used is given. On the right, the number of isotopes and their given labels. At the top, the subtitle is the [analysis.name] provided in worksheet 1.

3.2.3   Convex Hulls

The convex hull plots include the plot type "Isotopic Mixing Convex Hull" at the bottom. The title has the mixture name, followed by a title "Isotopic Signatures" that depends upon the information used to create it, possibly including modifiers such as "Discrimination Corrected. . . " and ". . . with Concentration Curves".

   A Convex Hull is the "rubber band" around the source points, it contains the set of points for which solutions exist for a mixture. Therefore, **(Important)** the mixture must fall within the Convex Hull of the sources for every pair of isotopes in order for solutions to exist. The Convex Hull plots show where the mixtures are relative to the sources they presumably consume, and the analysis gives higher proportions to sources close to a mixture and lower proportions to sources far from a mixture. When concentrations or assimilation efficiencies are specified, the convex hull will be curved to reflect this. Lines connecting all pairs of sources are plotted for reference, to help determine whether all sources are necessary to explain the diet, and to help understand the effect of concentration and assimilation efficiencies. When population variation is specified for the Isotope values, error bars appear on the points (but are not used in calculations).

3.2.4   One Mixture, pair of elements

Convex hull for one mixture and one pair of elements.
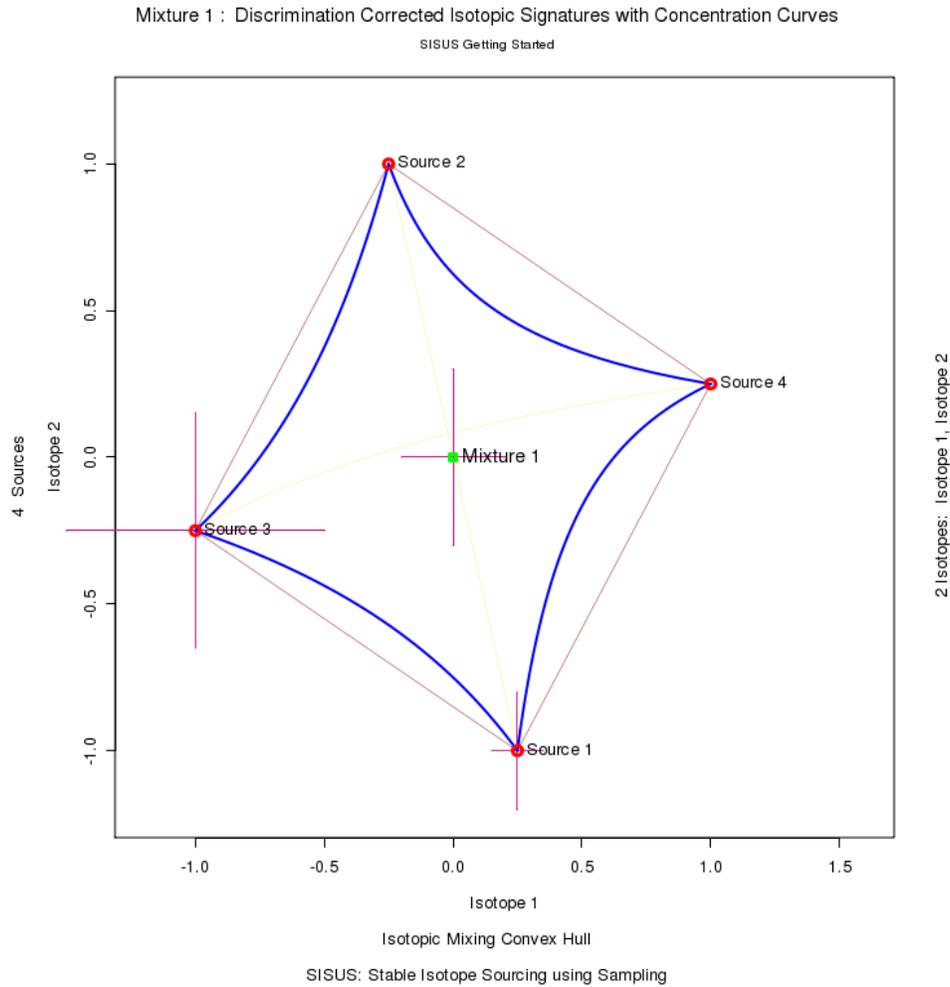
Figure 21: Convex Hull for Mixture 1, elements Isotope 1 and Isotope 2, file SISUS_GS_v0_08_plot_convex_hull_Mixture_1_Isotope_1_Isotope_2

3.2.5 One Mixture, matrix of all element pairs

Convex hull matrix for one mixture and all pairs of elements.
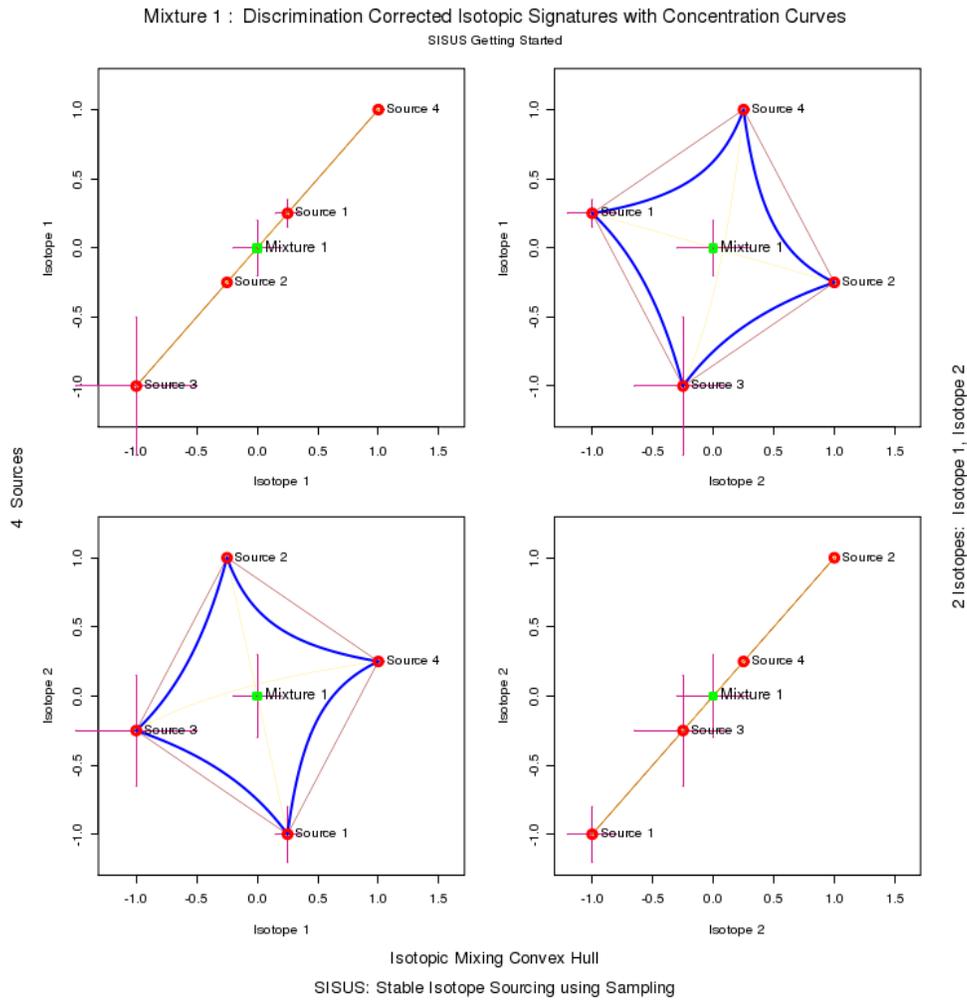
Figure 22: Convex Hull Matrix for Mixture 1, file SISUS_GS_v0_08_plot_convex_hull_matrix_Mixture_1

3.2.6   Mixture Group, pair of elements

Convex hull for mixture group and one pair of elements.
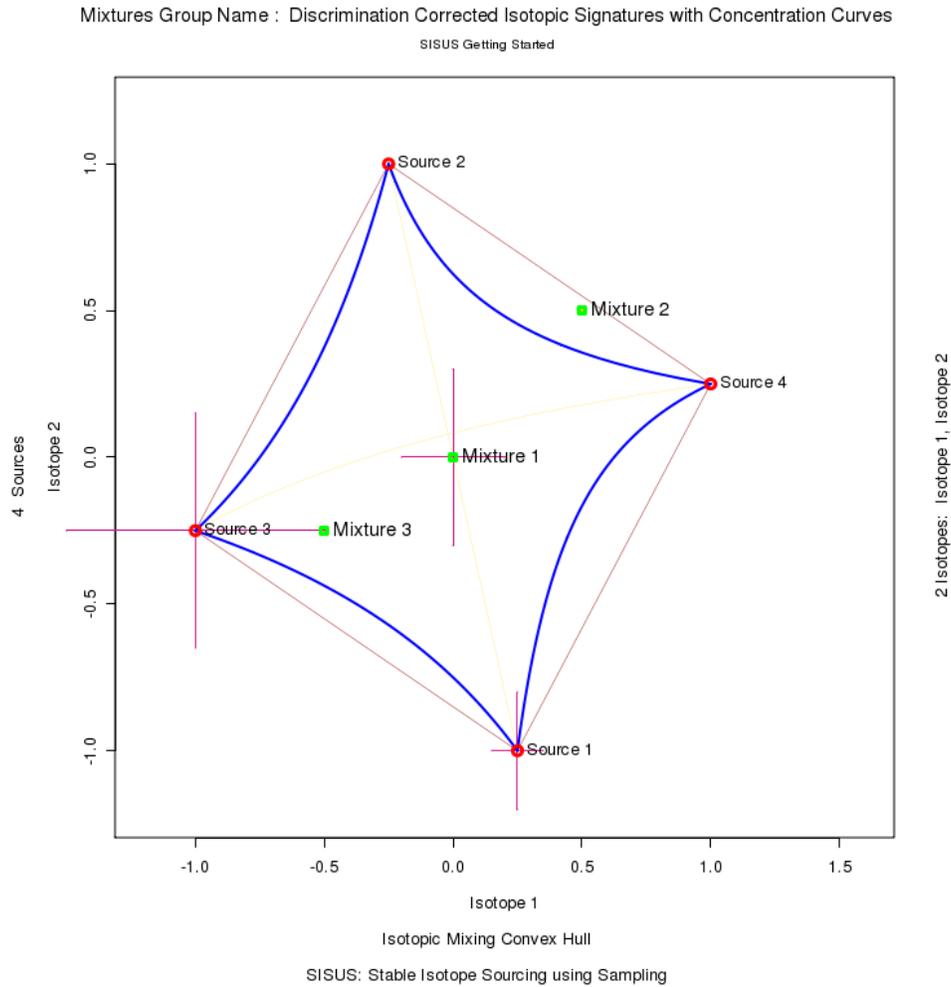
Figure   23:   Convex   Hull   for   Mixture   Group,
elements   Isotope   1   and   Isotope   2,   file
SISUS_GS_v0_08_plot_convex_hull_Mixtures_Group_Name_Isotope_1_Isotope_2

3.2.7   Mixture Group, matrix of all element pairs

Convex hull matrix for mixture group and all pairs of elements.
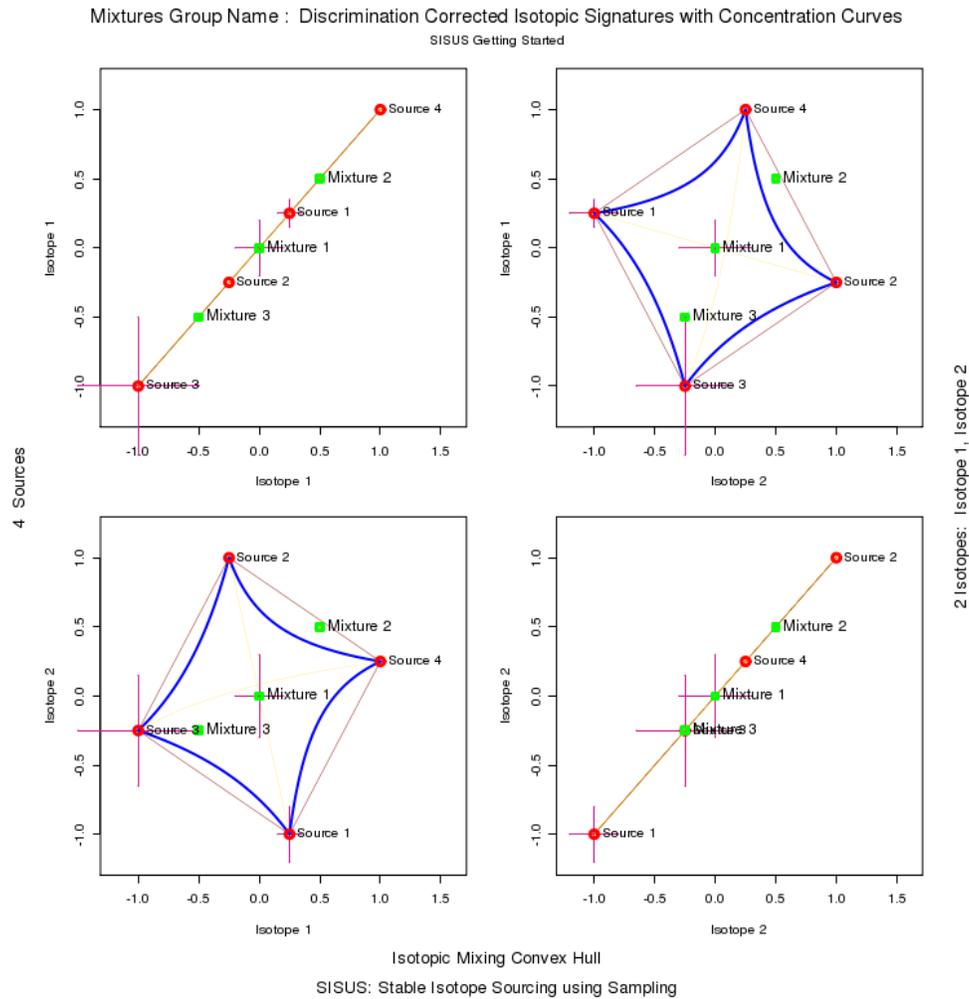
Figure 24: Convex Hull Matrix for Mixture Group, file SISUS_GS_v0_08_plot_convex_hull_matrix_Mixtures_Group_Name

3.2.8   Marginal Histograms

Marginal histograms with density smoothing curve for source proportions. The title shows that Biomass or an element is being plotted, and for the mixture name. If the density smoothing curve is overlayed, then it also shows the extent of the solutions (minimum and maximum).

Figure 25 on page 34 is for Biomass proportions. When concentrations or assimilation efficiencies are specified, plots for the proportion of each element would also be created. Figure 26 on page 35 is for Isotope 1 proportions and Figure 27 on page 36 is for Isotope 2 proportions.
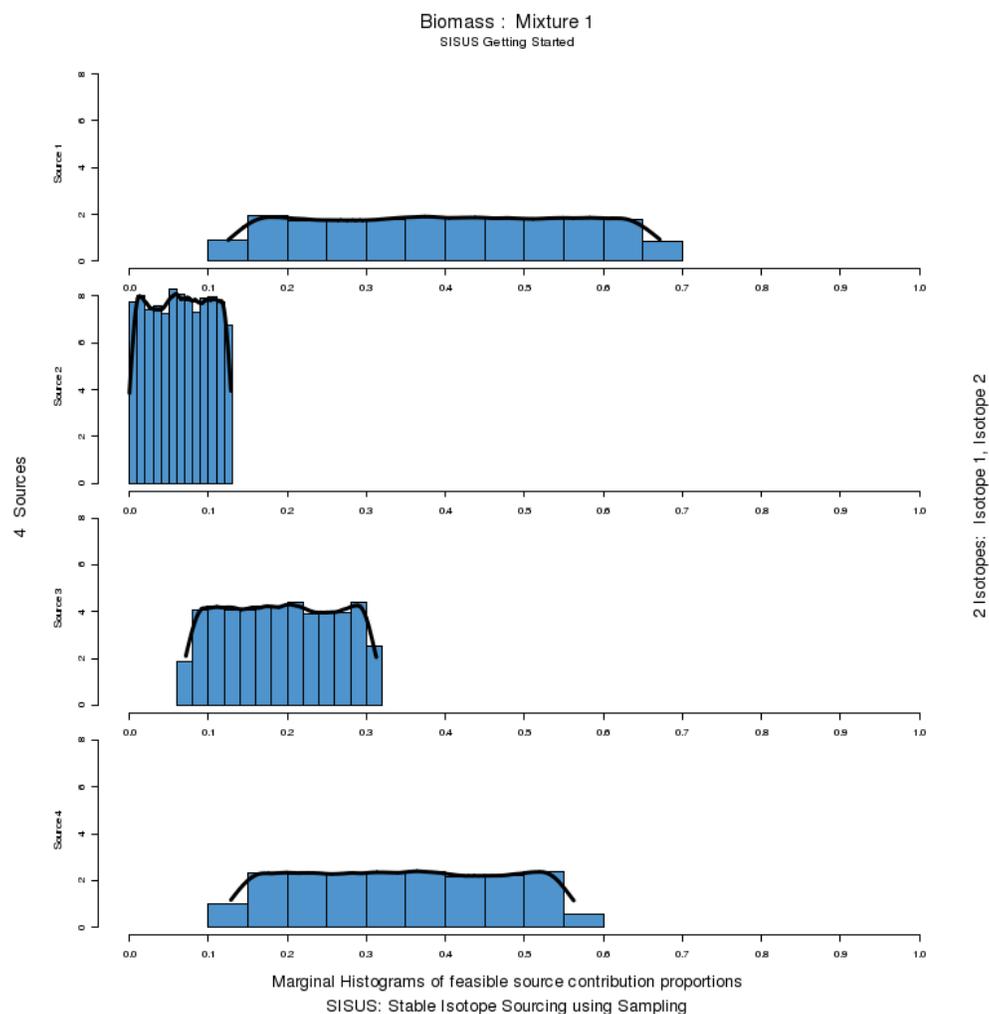
Figure 25: Marginal Histogram for Biomass for Mixture 1, file SISUS_GS_v0_08_plot_marginal_hist_unif_sam_Mixture_1_Biomass
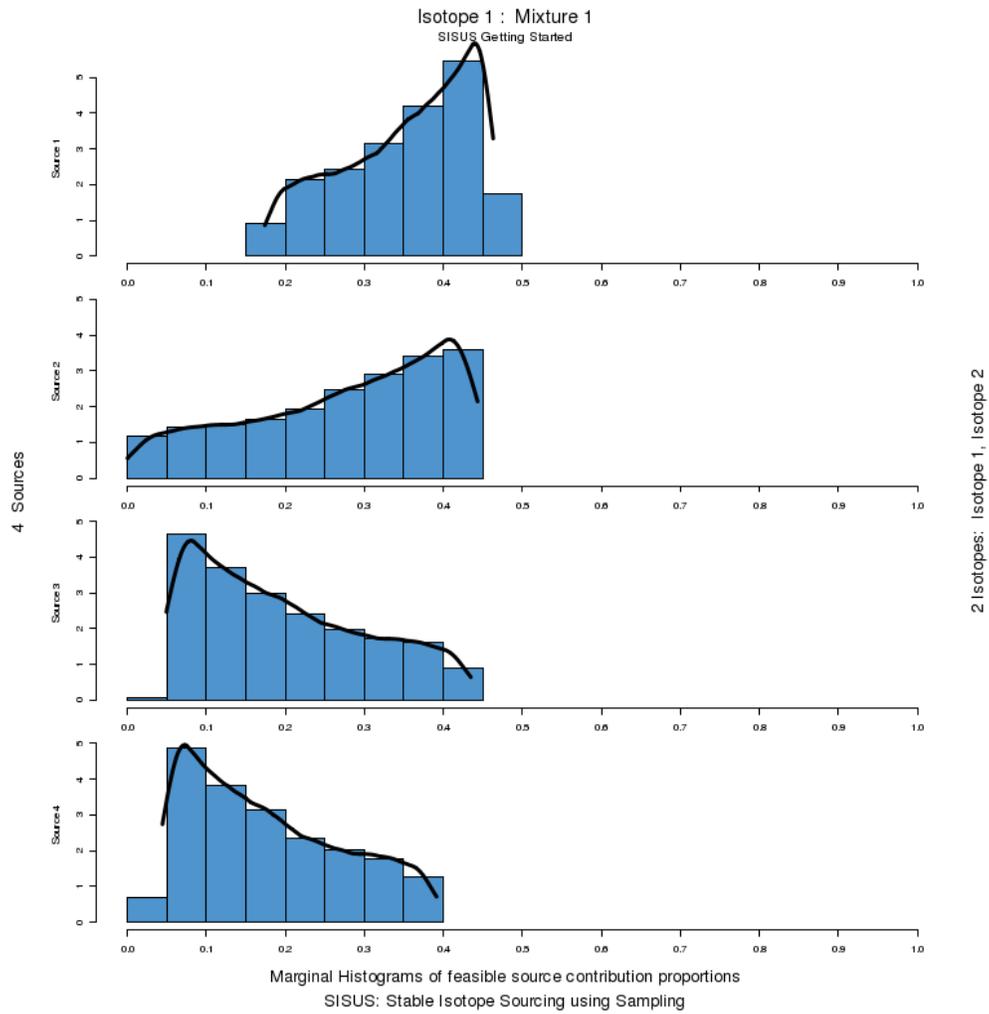
Figure 26: Marginal Histogram for Isotope 1 for Mixture 1, file SISUS_GS_v0_08_plot_marginal_hist_unif_sam_Mixture_1_Isotope_1
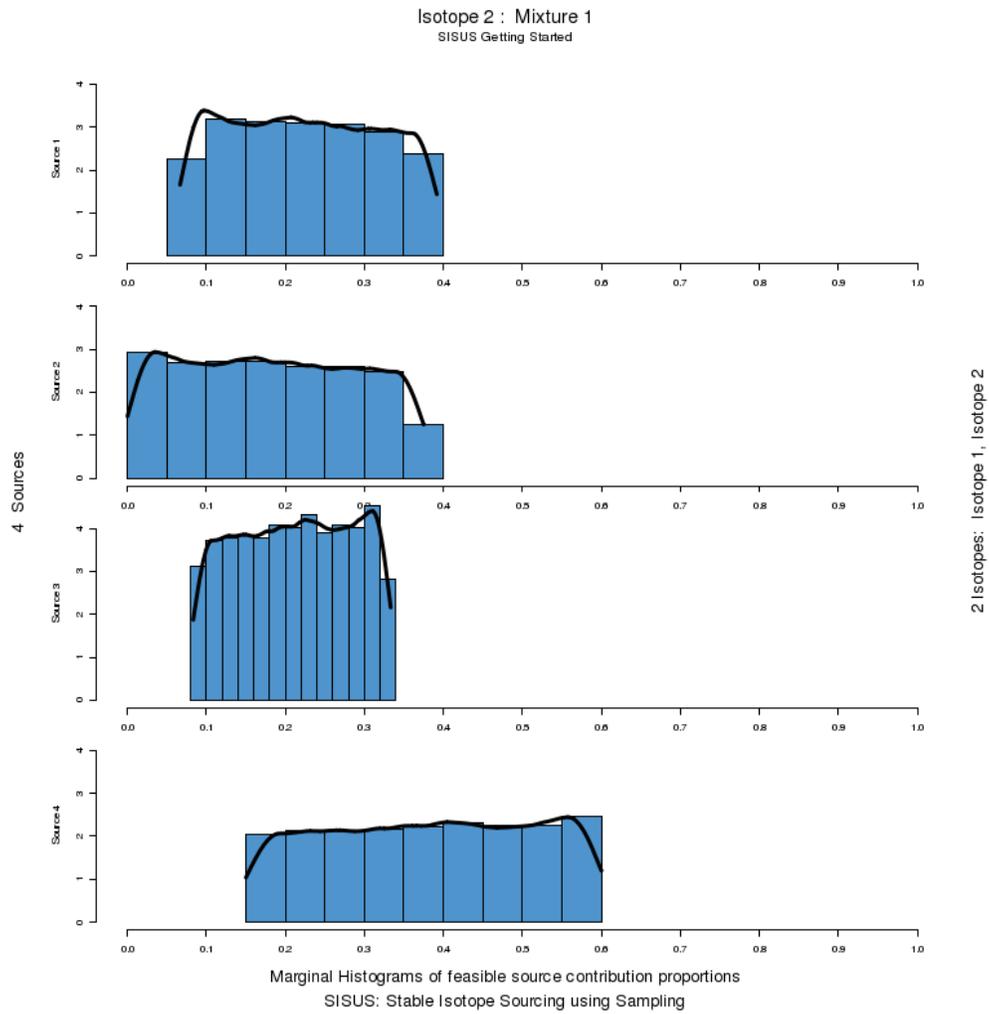
Figure 27: Marginal Histogram for Isotope 2 for Mixture 1, file SISUS_GS_v0_08_plot_marginal_hist_unif_sam_Mixture_1_Isotope_2

3.2.9 Statistics, Numerical Summaries

The table of statistics provides marginal summaries of the distribution of feasible solutions. The title gives credit to SISUS, and indicates Biomass or an element and for the mixture name. The [analysis.name] appears as a subtitle, defined in worksheet 1. The subsubtitle indicates whether these samples are the uniform sample or the Dirichlet resample.

The sources are columns and the statistics are rows. If there is a unique solution, a single row of numbers appear here identified "Unique". The first group of statistics are the moments of the distribution. The second group are the quantiles. The third group are pairs of endpoints for equal-tailed intervals.

The number of samples are M (or 1 if unique solution) defined on worksheet 1. The number of verticies for the solution polytope is given. The vertices are included to determine the min/max (and therefore range) values, but are not used in the sample for other summaries. The vertex points are given if specified, meant for advanced users who can make use of such information.

Figure 28 on page 38 gives the numerical summaries for the Uniform Sample Mixture 1. The first block is the Biomass proportions, followed by the proportion of each element.

Figure 29 on page 39 gives the numerical summaries for the Dirichlet Resample Mixture 1. The first block is the Biomass proportions, followed by the proportion of each element.

```
SISUS: Feasible Source Contributions of  Biomass to Mixture 1
       SISUS Getting Started
       Uniform Sample from Solution Polytope for Mixture 1

STATS        Source 1    Source 2    Source 3    Source 4
Mean         0.39905     0.06448     0.19159     0.34487
Sd           0.15778     0.03713     0.06961     0.12530
Var          0.02490     0.00138     0.00485     0.01570
Skewness    -0.01133    -0.01133     0.01133     0.01133
Kurtosis     1.80400     1.80400     1.80400     1.80400

Min          0.12500     0.00000     0.07143     0.12857
Q1           0.26179     0.03219     0.13106     0.23590
Median       0.40000     0.06471     0.19114     0.34406
Q3           0.53627     0.09677     0.25215     0.45387
Max          0.67143     0.12857     0.31250     0.56250
Range        0.54643     0.12857     0.24107     0.43393
IQR          0.27448     0.06458     0.12109     0.21797

CIL80        0.17937     0.01279     0.09546     0.17184
CIU80        0.61695     0.11575     0.28851     0.51933
CIL90        0.15316     0.00663     0.08324     0.14983
CIU90        0.64465     0.12227     0.30007     0.54013
CIL95        0.13917     0.00333     0.07740     0.13933
CIU95        0.65791     0.12539     0.30629     0.55132
CIL98        0.13061     0.00132     0.07404     0.13327
CIU98        0.66554     0.12719     0.31004     0.55807
CIL99        0.12783     0.00067     0.07275     0.13094
CIU99        0.66848     0.12788     0.31125     0.56025

Samples      10000

Solution Polytope Vertices  2
             0.67143     0.12857     0.07143     0.12857
             0.12500     0.00000     0.31250     0.56250


SISUS: Feasible Source Contributions of  Isotope 1 to Mixture 1
       SISUS Getting Started
       Uniform Sample from Solution Polytope for Mixture 1

STATS        Source 1    Source 2    Source 3    Source 4
Mean         0.35216     0.27330     0.19713     0.17741
Sd           0.08083     0.12394     0.10778     0.09700
...

SISUS: Feasible Source Contributions of  Isotope 2 to Mixture 1
       SISUS Getting Started
       Uniform Sample from Solution Polytope for Mixture 1

STATS        Source 1    Source 2    Source 3    Source 4
Mean         0.22481     0.18248     0.21168     0.38103
Sd           0.09379     0.10822     0.07215     0.12987
...
```

Figure 28: Numerical Summaries, SISUS_GS_v0_08_sisus_stats_Mixture_1.txt (Uniform Samples)

```
SISUS: Feasible Source Contributions of  Biomass to Mixture 1
       SISUS Getting Started
       Dirichlet Resample from Solution Polytope for Mixture 1

STATS          Source 1   Source 2   Source 3   Source 4
Mean           0.23564    0.02603    0.26369    0.47464
Sd             0.12964    0.03050    0.05719    0.10295
Var            0.01681    0.00093    0.00327    0.01060
Skewness       1.37386    1.37386   -1.37386   -1.37386
Kurtosis       4.00362    4.00362    4.00362    4.00362

Min            0.12500    0.00000    0.07143    0.12857
Q1             0.13695    0.00281    0.23783    0.42809
Median         0.18039    0.01303    0.28802    0.51844
Q3             0.29426    0.03983    0.30723    0.55301
Max            0.67143    0.12857    0.31250    0.56250
Range          0.54643    0.12857    0.24107    0.43393
IQR            0.15731    0.03701    0.06940    0.12492

CIL80          0.12707    0.00049    0.17283    0.31109
CIU80          0.44159    0.07449    0.31159    0.56086
CIL90          0.12573    0.00017    0.13460    0.24228
CIU90          0.52824    0.09488    0.31218    0.56192
CIL95          0.12532    0.00007    0.11106    0.19991
CIU95          0.58189    0.10750    0.31236    0.56225
CIL98          0.12506    0.00001    0.09119    0.16414
CIU98          0.62711    0.11814    0.31247    0.56245
CIL99          0.12506    0.00001    0.08198    0.14756
CIU99          0.64795    0.12305    0.31247    0.56245

Samples        10000

Solution Polytope Vertices  2
               0.67143    0.12857    0.07143    0.12857
               0.12500    0.00000    0.31250    0.56250


SISUS: Feasible Source Contributions of  Isotope 1 to Mixture 1
       SISUS Getting Started
       Dirichlet Resample from Solution Polytope for Mixture 1

STATS          Source 1   Source 2   Source 3   Source 4
Mean           0.25595    0.12580    0.32540    0.29286
Sd             0.08062    0.12362    0.10749    0.09675
...

SISUS: Feasible Source Contributions of  Isotope 2 to Mixture 1
       SISUS Getting Started
       Dirichlet Resample from Solution Polytope for Mixture 1

STATS          Source 1   Source 2   Source 3   Source 4
Mean           0.12945    0.07244    0.28504    0.51307
Sd             0.07523    0.08681    0.05787    0.10417
...
```

Figure 29: Numerical Summaries, SISUS_GS_v0_08_sisus_stats_Mixture_1.txt (Dirichlet Resamples)

3.2.10   Samples

Uniform samples and Dirichlet resamples are provided in comma seperated
values (csv) files, which can be easily read into spreadsheet programs. This
allows an advanced user to perform their own analysis using the samples.
The first column identifies whether this is the Uniform Sample "sam" or the
Dirichlet Resamples "resam", with an observation number. The columns are
labelled a Biomass group, then Element groups for all the sources.

Figure 30 on page 40 gives the first 10 Uniform Samples for Mixture 1.
Figure 31 on page 40 gives the first 10 Dirichlet Resamples for Mixture 1.

```
"sam","BiomasSource 1","BiomasSource 2","BiomasSource 3","BiomasSource 4","Isotope 1_Source 1","Isotope 1_Source 2","Is
1,0.175124732790819,0.0117940547743014,0.290386147298179,0.522695065136735,0.222853575840266,0.075042149621679,0.369528
2,0.474222561847655,0.0821700145523672,0.158431222714272,0.285176200885721,0.399819388996282,0.346389729794184,0.133574
3,0.540165699851334,0.0976860470238206,0.129338661830295,0.232809591294566,0.423878994130184,0.383281124332840,0.101494
4,0.125711522337949,0.000167417020670008,0.312186093086212,0.5619349675552,0.174671586497026,0.00116309929524288,0.4337
5,0.494620695615463,0.0869695754389088,0.149432046052014,0.268977682893645,0.407635562855118,0.358374529711064,0.123152
6,0.658298714366705,0.125482050439201,0.0772211554264657,0.138998079767657,0.459568076306078,0.438004383669222,0.053909
7,0.573709700842064,0.105578753139285,0.114539837863809,0.206171708154878,0.434882519958246,0.400153197269201,0.0868233
8,0.141330194237212,0.00384239864402561,0.30529550254242,0.549531904576379,0.190831081792415,0.0259409920815085,0.41222
9,0.227954367656424,0.0242245570956049,0.267078955445709,0.480742119802298,0.266137930056096,0.141411492752513,0.311816
10,0.439275828975219,0.0739472538765012,0.173848898981540,0.312928018166827,0.385557963266762,0.324522210342268,0.15258
```

Figure 30: Uniform Samples, SISUS_GS_v0_08_sisus_samples_Mixture_1.txt

```
"resam","BiomasSource 1","BiomasSource 2","BiomasSource 3","BiomasSource 4","Isotope 1_Source 1","Isotope 1_Source 2","
1,0.184877220816237,0.0140887578386217,0.286083579052518,0.514950442303957,0.231420569718428,0.0881782068997993,0.35810
2,0.322563147840672,0.0464854465506185,0.225339787716988,0.405611617901337,0.32809616909676,0.236414125948814,0.2292051
3,0.224883484404928,0.0235019963305323,0.268433756879908,0.483180762394356,0.263818442174498,0.137854944668759,0.314908
4,0.147987986496995,0.00540893799960533,0.302358241252349,0.544244834254015,0.197445435072610,0.0360830004479633,0.4034
5,0.401002727492173,0.0649418182342969,0.190734090812694,0.343321363463158,0.368532578271593,0.29841662002159,0.1752898
6,0.242315084230326,0.0276035492309429,0.260743345193441,0.469338021347588,0.276695879160131,0.157600348047995,0.297738
7,0.129925547447119,0.00115895234050462,0.310326964361364,0.558588535860965,0.179123268176416,0.00798901120568254,0.427
8,0.128732184288888,0.000878161009017145,0.310853448107468,0.559536206604295,0.177869644663055,0.00606678848392352,0.42
9,0.382405902674908,0.0605660947475811,0.198938572349946,0.358089430230339,0.359667823749743,0.284823996419873,0.187109
10,0.289592649304935,0.0387276821919432,0.239885595895798,0.43179407262632,0.308400880227925,0.206214683035794,0.255465
```

Figure 31: Dirichlet Resamples, SISUS_GS_v0_08_sisus_samples_Mixture_1.txt

3.2.11   Scatterplot Matrix

Scatterplot matrix with two-dimensional density estimation. The title shows the mixture name and whether the uniform samples or Dirichlet resamples are plotted.

The diagonal includes the marginal histograms for each source. The upper triangle includes the sample points and density smoothing. The lower triangle includes only the density smoothing. The darker the density, the more points are there.

Figure 32 on page 42 shows the Biomass Uniform Samples for Mixture 1. Figure 33 on page 43 shows the Isotope 1 Uniform Samples for Mixture 1. Figure 34 on page 44 shows the Biomass Dirichlet Resamples for Mixture 1. Figure 35 on page 45 shows the Isotope 1 Dirichlet Resamples for Mixture 1.
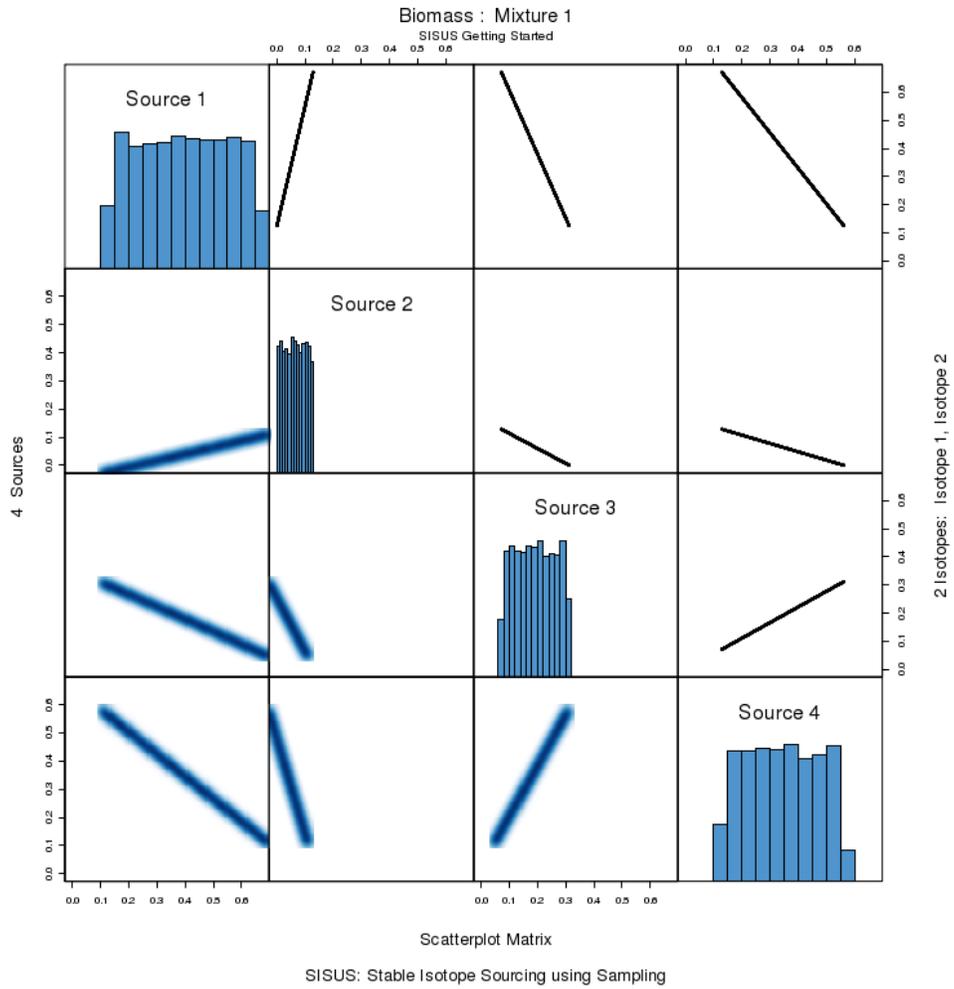
Figure 32: Scatterplot matrix, Uniform Samples, file SISUS_GS_v0_08_plot_scatterplot_matrix_unif_sam_Mixture_1_Biomass

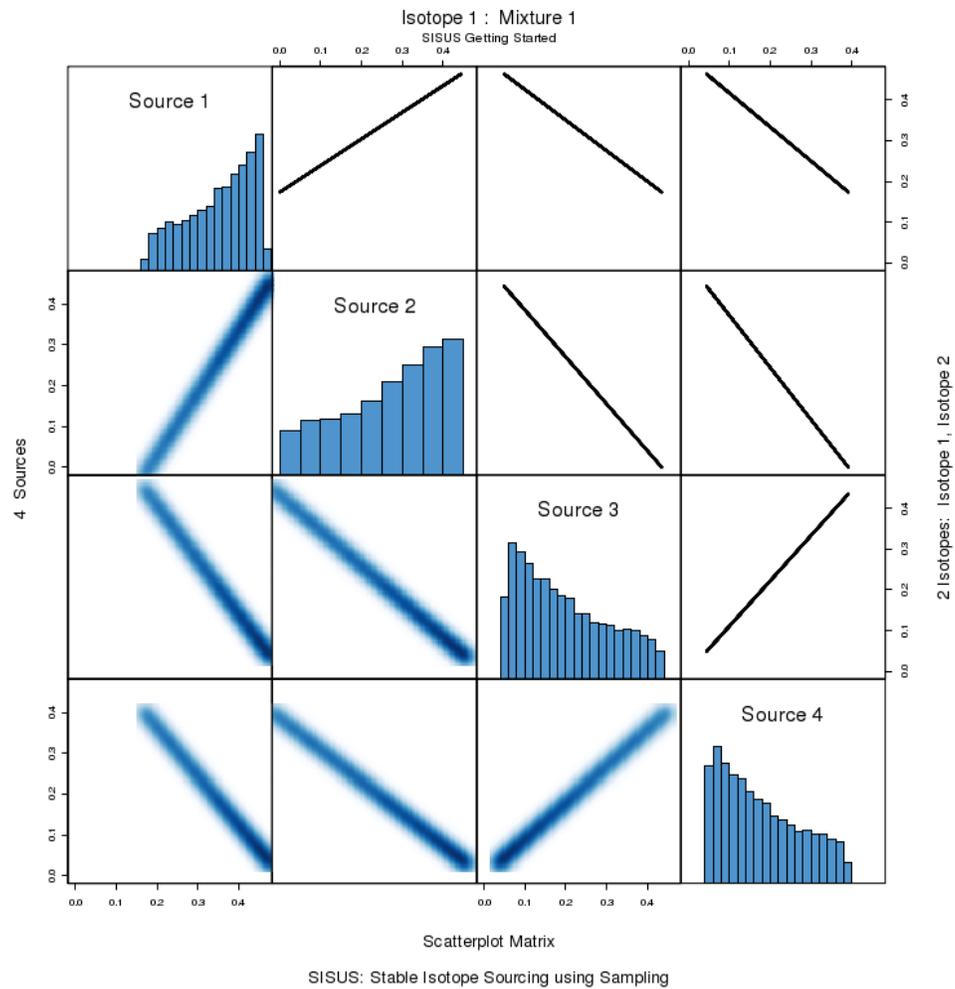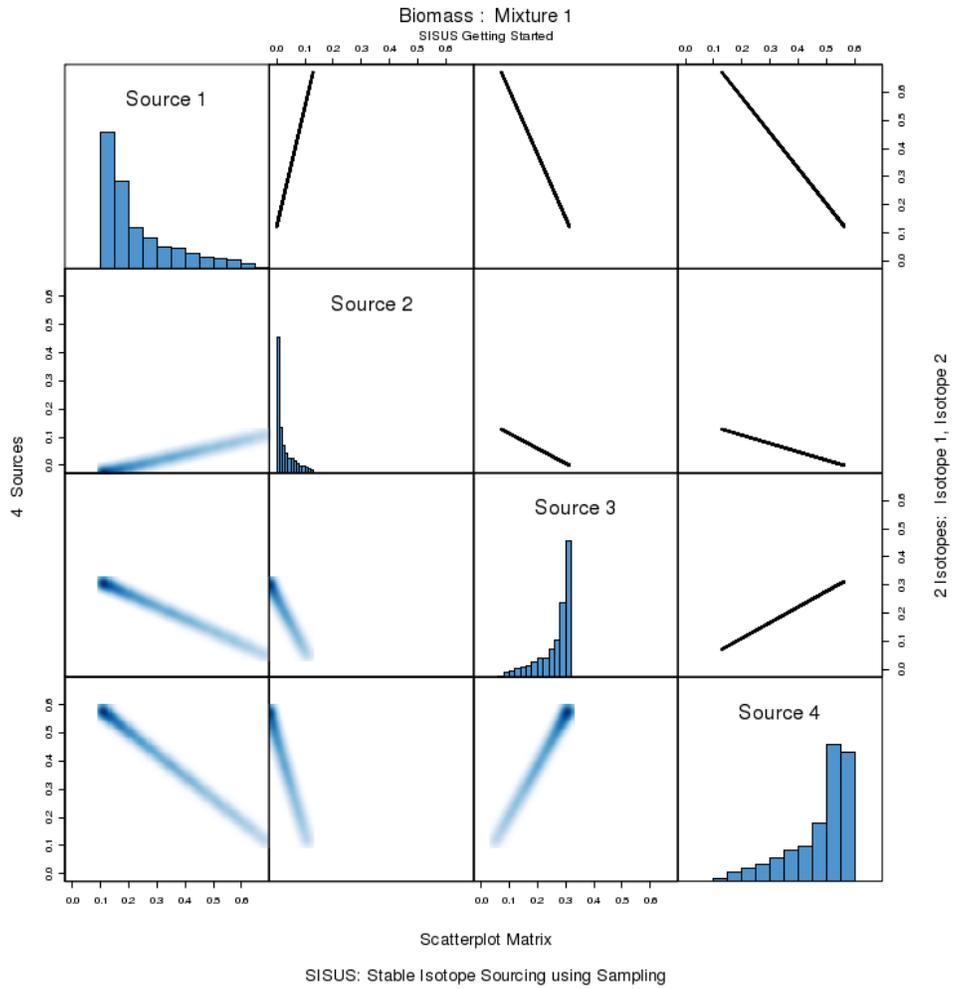Figure 33: Scatterplot matrix, Uniform Samples, file SISUS_GS_v0_08_plot_scatterplot_matrix_unif_sam_Mixture_1_Isotope_1

Figure 34: Scatterplot matrix, Dirichlet Resamples, file SISUS_GS_v0_08_plot_scatterplot_matrix_dir_resam_Mixture_1_Biomass
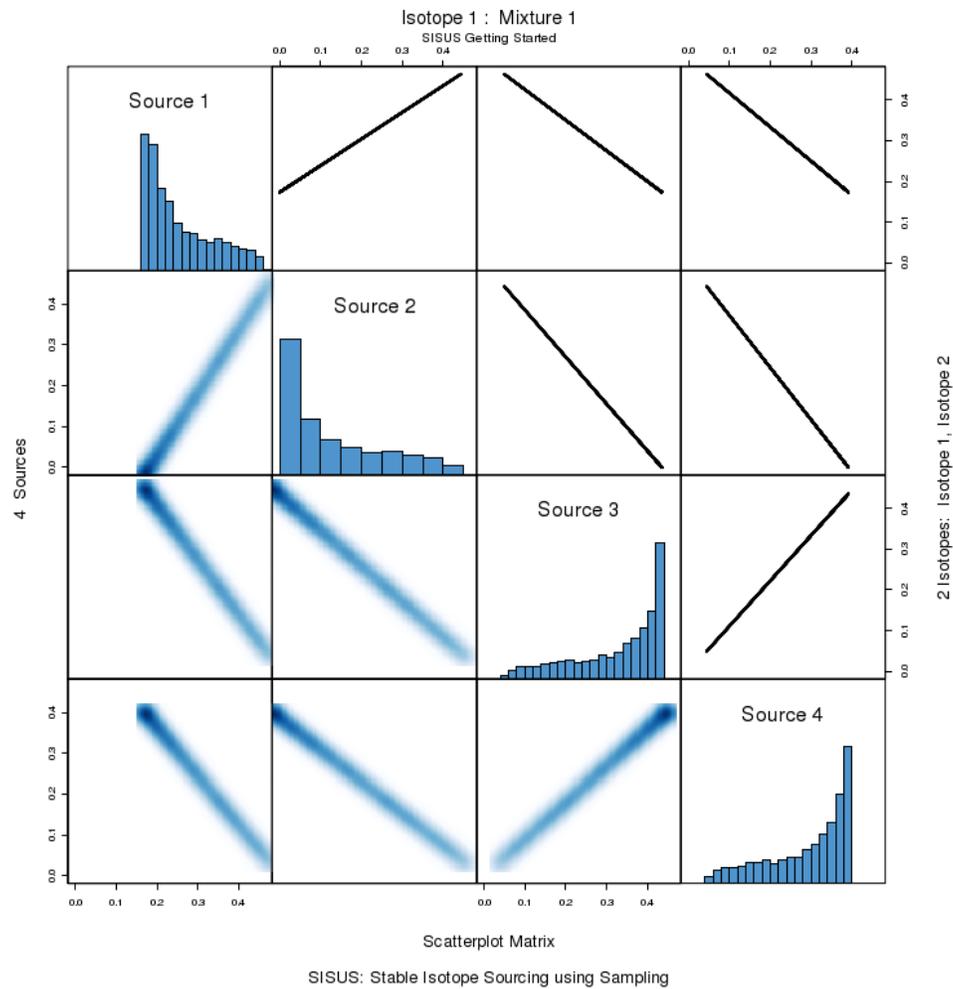
Figure 35: Scatterplot matrix, Dirichlet Resamples, file SISUS_GS_v0_08_plot_scatterplot_matrix_dir_resam_Mixture_1_Isotope_1