

# SISUS: Stable Isotope Sourcing using Sampling Getting Started

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May 30, 2007

S<sup>TABLE</sup> I<sup>SOTOPE</sup> S<sup>SOURCING</sup> U<sup>SING</sup> S<sup>SAMPLING</sup>

<http://StatAcumen.com/sisus>

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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, either by email or on SISUSWiki.

Regards,  
Erik Barry Erhardt

# 1 Overview

**SISUS**: Stable Isotope Sourcing using Sampling is a Bayesian statistical model and software aiming to provide a comprehensive solution to stable isotope sourcing inference and prediction problems. **SISUS** has been designed to solve the most detailed models to date. **SISUS** uses a single Excel workbook as an input file to submit to the **SISUS** website, <http://StatAcumen.com/sisus>. 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 11 (v.0.08) 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. A template **SISUS** Excel workbook is available for download from <http://StatAcumen.com/sisus>, as well as many examples to try.

## 1.1 Procedure for execution

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

1. Visit <http://StatAcumen.com/sisus> and download the Workbook from the menu bar.
2. Input your data in the Workbook, setting the parameter values that correspond to your desired analysis.
3. Upload the workbook at the Execute page in the menu bar.
4. Follow the results link to the output of the program, available as descriptive filenames.
5. If desired, download the zip archive file of all results and the submitted data file for use in publication or report.

## 1.2 SISUS website

SISUS is located at <http://StatAcumen.com/sisus>. Figure 1 on page 4 shows the top of the website. In particular, observe the menu to the left.

**Execute:** the submission page when the completed workbook is uploaded; described in section 3, with the results described in section 4.

**Workbook:** downloads `SISUS_v0_08_template.xls`, the current workbook for data input; the format of this workbook is described in the next section 2.

**Getting Started:** this document.

**Examples:** the Workbooks and SISUS outputs from published studies, with complete citations and brief description of the study's modelling characteristics.

**SISUSBugs:** the location at **SISUSWiki** for reporting problems or suggesting features or enhancements.

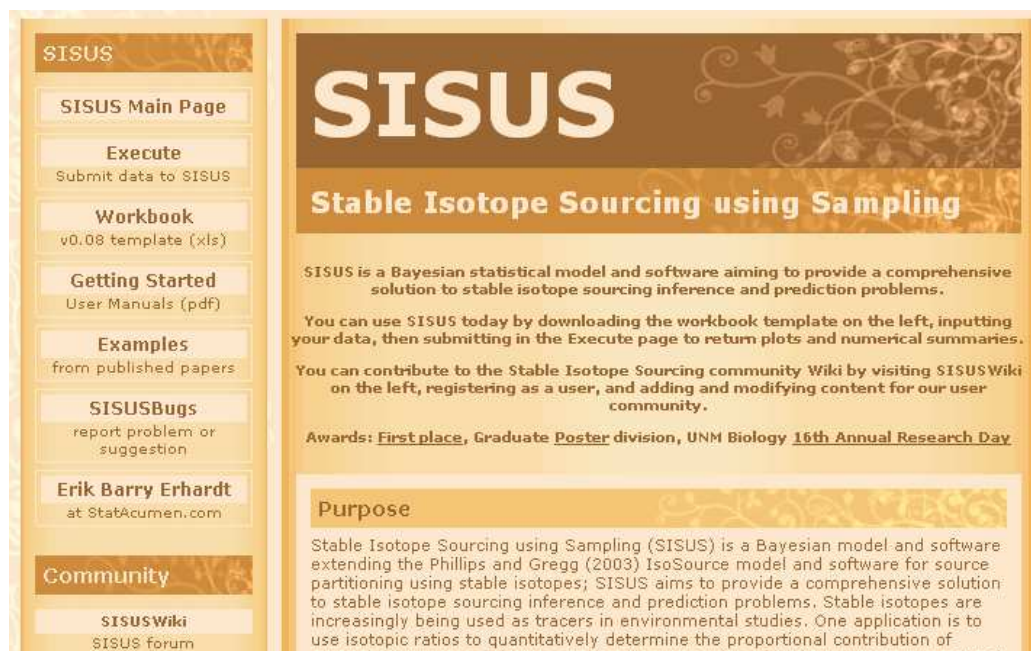


Figure 1: SISUS website at <http://StatAcumen.com/sisus>

## 2 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.

## 2.1 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	<b>SISUS Parameters</b>	<b>Settings</b>	<b>Values</b>
2	<b>Analysis Labels</b>	<i>SISUS v0.08</i>	<b>Description</b>
3	analysis.name	<b>SISUS Getting Started</b>	<i>long text</i> name of this analysis to print on plots and tables
4	filename.prefix	<i>SISUS_GS_v0_08</i>	<i>short string</i> character string (no spaces) at beginning of all output filenames (if blank, default is "SISUS")
5	mixtures.group.name	Mixtures Group Name	<i>short string</i> If n.mixtures > 1, then name the group of mixtures
6	<b>Data Dimensions</b>		
7	n.mixtures	3	<i>1 or more</i> number of mixtures to analyze together
8	n.sources	4	<i>2 or more</i> n = number of sources composing the mixture
9	n.isotopes	2	<i>1 or more</i> k = number of isotopes measured
10	<b>Sampling</b>		
11	M	10000	<i>10000 or so</i> total number of samples to retain
12	skip	100	<i>100 or so</i> draw [skip] samples from the polytope keeping the last one
13	burnin	10	<i>10 or so</i> number of samples to draw to get off the boundary of the polytope (there is a check to guarent
14	seed	76643	<i>0-100000</i> random seed (to repeat results)
15	<b>Mixing Model</b>		
16	simplex.include.sw	1	<i>(1=use, 0=ignore)</i> Include simplex constraint (1=yes, usually estimating proportion of diet, 0=no, estimating fract
17	discrimination.include.sw	1	<i>(1=use, 0=ignore)</i> Correct for discrimination using values on Discrimination worksheet (Source Isotopic Values +
18	concentration.include.sw	1	<i>(1=use, 0=ignore)</i> Include concentration dependence
19	assimeffic.include.sw	0	<i>(1=use, 0=ignore)</i> Include assimilation efficiency
20	lc.include.sw	1	<i>(1=use, 0=ignore)</i> Use defined Linear Constraints
21	prior.include.sw	1	<i>(1=use, 0=ignore)</i> Resample uniform sampe based on defined Dirichlet distribution
22	isotope.stddev.include.sw	1	<i>(1=use, 0=ignore)</i> Isotope standard deviations used for error bars on convex hull plots
23	biomass.per.individual.include.sw	0	<i>(1=use, 0=ignore)</i> Use Biomass per Individual and Number of Individuals in Proportions of Source Consumed mo
24	<b>Output Settings</b>		
25	plot.convex.hull.include.sw	1	<i>(1=make, 0=don't)</i> Output Convex Hull plot
26	plot.marginal.histogram.include.sw	1	<i>(1=make, 0=don't)</i> Output Marginal Histogram plot
27	plot.scatterplot.matrix.include.sw	1	<i>(1=make, 0=don't)</i> Output Scatterplot Matrix
28	numerical.summaries.include.sw	1	<i>(1=make, 0=don't)</i> Output Numerical Summaries and Statistics
29	solution.polytope.vertices.sw	1	<i>(1=make, 0=don't)</i> Output solution polytope vertices as part of numerical summary
30	samples.include.sw	1	<i>(1=make, 0=don't)</i> Output solution polytope samples
31	time.series.sw	0	<i>(1=make, 0=don't)</i> Output list of means for multiple mixtures as a series over time
32	hist.bins	10	<i>10</i> number of bins for histograms in marginal histogram plots
33	hist.density.sw	1	<i>(1=use, 0=ignore)</i> Overlay a density smoother on the marginal histogram plots
34	<b>Plot Formats</b>		
35	plot.type.png	1	<i>(1=make, 0=don't)</i> produce plots in (.png) Portable Network Graphics format (0=no, 1=yes) (lossless for web) (A
36	plot.type.eps	1	<i>(1=make, 0=don't)</i> produce plots in (.eps) Encapsulated PostScript format (0=no, 1=yes) (for LaTeX and "nix)
37	plot.type.pdf	0	<i>(1=make, 0=don't)</i> produce plots in (.pdf) Portable Document Format format (0=no, 1=yes) (for pdfLaTeX)
38	plot.type.bmp	0	<i>(1=make, 0=don't)</i> produce plots in (.bmp) Windows and OS/2 bitmap format (0=no, 1=yes) (for Windows)
39	plot.type.jpeg	0	<i>(1=make, 0=don't)</i> produce plots in (.jpeg) Joint Photographic Experts Group format (0=no, 1=yes) (compressed)
40	plot.type.gif	0	<i>(1=make, 0=don't)</i> produce plots in (.gif) Graphics Interchange Format (0=no, 1=yes) (compressed)
41			
42			<b>Color Key:</b>
43			<b>Worksheet Titles</b>
44			Unchangable Cells
45			Changeable Cells, for "no effect" or "default"
46			Changeable Cells, for "effect" or "setting"
47			"Proportions of Sources Consumed Mixing Model" does not use Simplex

Figure 2: Worksheet 1, SISUS Parameters

### 2.1.1 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	<b>SISUS Parameters</b>	<b>Settings</b>	<b>Values</b>
2	<b>Analysis Labels</b>	<i>SISUS v0.08</i>	
3	analysis.name	SISUS Getting Started	<i>long text</i>
4	filename.prefix	SISUS_GS_v0_08	<i>short string</i>
5	mixtures.group.name	Mixtures Group Name	<i>short string</i>

Figure 3: Worksheet 1, SISUS Parameters: Analysis Labels

### 2.1.2 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	<b>Data Dimensions</b>		
7	n.mixtures	3	1 or more
8	n.sources	4	2 or more
9	n.isotopes	2	1 or more

Figure 4: Worksheet 1, SISUS Parameters: Data Dimensions

### 2.1.3 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	<b>Sampling</b>		
11	M	10000	10000 or so
12	skip	100	100 or so
13	burnin	10	10 or so
14	seed	76543	0-100000

Figure 5: Worksheet 1, SISUS Parameters: Sampling

### 2.1.4 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	<b>Mixing Model</b>	
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 6: Worksheet 1, SISUS Parameters: Mixing Model

### 2.1.5 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 vertices 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	<b>Output Settings</b>		
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 7: Worksheet 1, SISUS Parameters: Output Settings

### 2.1.6 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,  $\text{\LaTeX}$  users might output vector formats eps and pdf (for  $\text{\LaTeX}$  and pdf $\text{\LaTeX}$ ), 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	<b>Plot Formats</b>		
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 8: Worksheet 1, SISUS Parameters: Plot Formats

### 2.1.7 Worksheet 1, SISUS Parameters: Color Key

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

**Orange** Used for titles of worksheets.

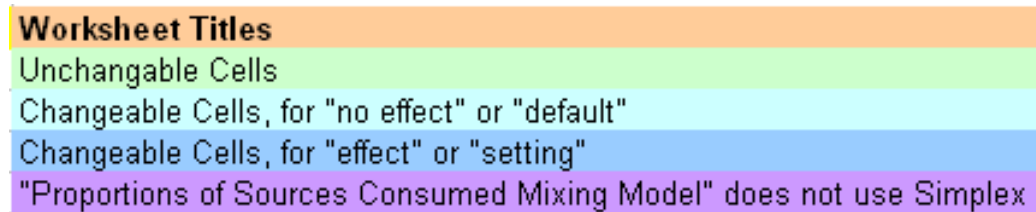
**Green** Cells that are information only, not used as SISUS input.

**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.



<b>Worksheet Titles</b>
Unchangeable Cells
Changeable Cells, for "no effect" or "default"
Changeable Cells, for "effect" or "setting"
"Proportions of Sources Consumed Mixing Model" does not use Simplex

Figure 9: Worksheet 1, SISUS Parameters: Color Key

## 2.2 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  $j = 1, \dots, k$  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	<b>Mixtures Isotopic Values</b>	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 10: Worksheet 2, Mixtures Isotope Ratios

## 2.3 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  $i = 1, \dots, n$  sources and  $j = 1, \dots, k$  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	<b>Sources Isotopic Values</b>	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 11: Worksheet 3, Sources Isotope Ratios

## 2.4 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	<b>Sources Discrimination</b>	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 12: Worksheet 4, Sources Discrimination

## 2.5 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 dependent 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	<b>Sources Concentration</b>	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 13: Worksheet 5, Sources Concentration

## 2.6 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 assimilation efficiency concentration dependent 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	<b>Sources Assimilation Efficiency</b>	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 14: Worksheet 6, Sources Assimilation Efficiency

## 2.7 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  $1p_1 + 2p_2 + \dots + np_n = b$ , where  $\{1, 2, \dots, n\}$  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.

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

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

	A	B	C	D	E	F
1	<b>Linear Constraints</b>	Equal	Minimum	Maximum	GE	
2	RHS b				0.00	
3	Source 1					
4	Source 2				-1.00	
5	Source 3					
6	Source 4				1.00	
7	0					
8	0					
9	0					
10	0					

Figure 15: Worksheet 7, Linear Constraints: Showing Source 4  $\geq$  Source 2

## 2.8 Worksheet 8, Prior

Worksheet 8 is used for incorporating prior information (expert opinion) on source proportion vector  $p_B$ . The simplex is the constraint that the sum of the source proportions is 1. 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	<b>Priors</b>	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 16: Worksheet 8, Priors

## 2.9 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	<b>Mixtures Isotope StdDev</b>	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 17: Worksheet 9, Mixtures Isotope StdDev

## 2.10 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	<b>Sources Isotope StdDev</b>	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 18: Worksheet 10, Sources Isotope StdDev

## 2.11 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),  $B_i = BPI_i \times NCI_i$ .

	A	B	C	D	E	F
1	<b>Sources Biomass per Individual</b>	<b>Biomass</b>	<b>Number</b>			
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 19: Worksheet 11, Sources Biomass per Individual

## 3 Execute

### 3.1 Submit Workbook

Choosing **Execute** from the SISUS website menu will bring you to a page where you can upload your completed workbook for analysis. Click the “Browse...” button, locate the workbook on your computer, then click “Analyse”<sup>1</sup>.

## SISUS: Stable Isotope Sourcing using Sampling

SISUS is a Bayesian statistical model and software aiming to provide a comprehensive solution to stable isotope sourcing inference and prediction problems. <http://statacumen.com/sisus/>



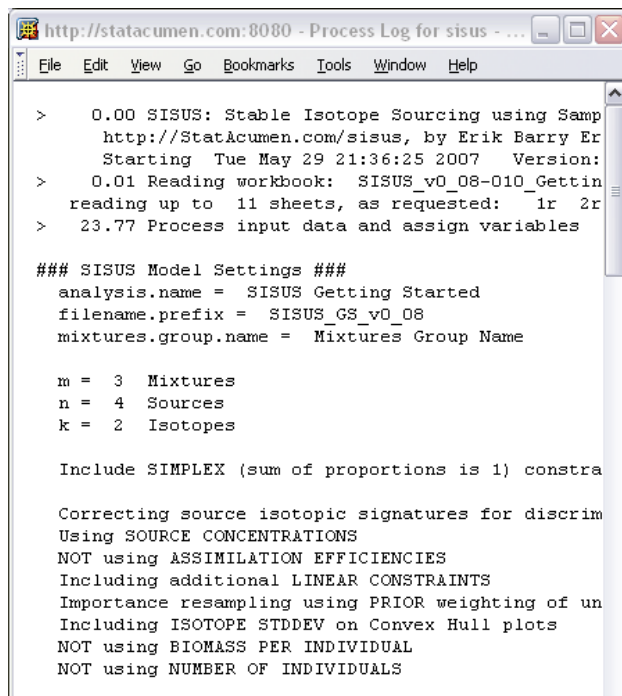
Upload SISUS Excel workbook for analysis

Figure 20: Website Execute: Upload page

<sup>1</sup>British English because this interface is RWUI, developed by Richard Newton at <http://rwui.cryst.bbk.ac.uk/>

## 3.2 Process Log

Upon submission, a Process Log window will open and refresh every 5 seconds or so. This will let you know what SISUS is currently working on.



```
> 0.00 SISUS: Stable Isotope Sourcing using Samp
http://StatAcumen.com/sisus, by Erik Barry Er
Starting Tue May 29 21:36:25 2007 Version:
> 0.01 Reading workbook: SISUS_v0_08-010_Gettin
reading up to 11 sheets, as requested: 1r 2r
> 23.77 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

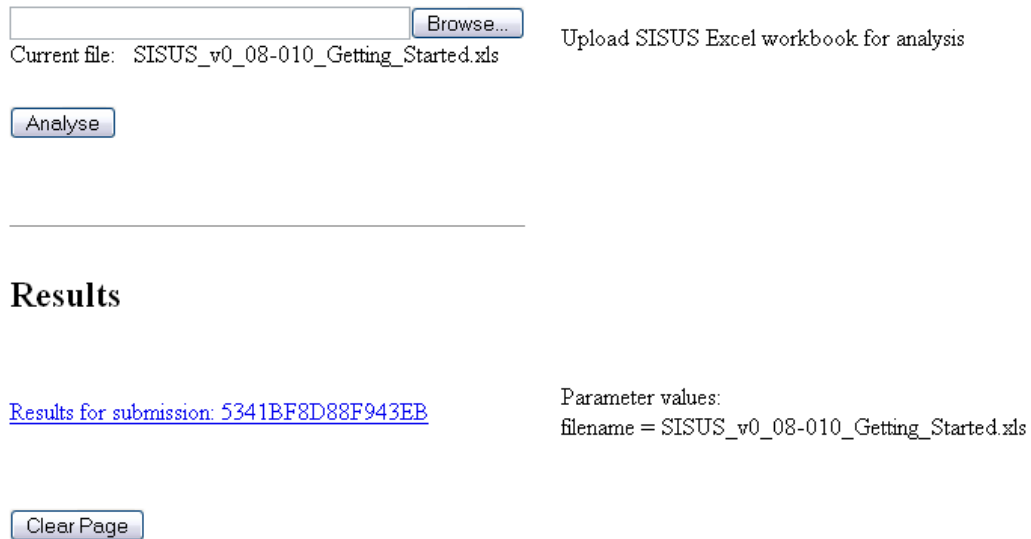
Include SIMPLEX (sum of proportions is 1) constra

Correcting source isotopic signatures for discrim
Using SOURCE CONCENTRATIONS
NOT using ASSIMILATION EFFICIENCIES
Including additional LINEAR CONSTRAINTS
Importance resampling using PRIOR weighting of un
Including ISOTOPE STDDEV on Convex Hull plots
NOT using BIOMASS PER INDIVIDUAL
NOT using NUMBER OF INDIVIDUALS
```

Figure 21: Website Execute: Process Log window

### 3.3 Results List

When SISUS completes, the initial window will refresh, and the **Results** section will appear at the bottom of the page. Each submission is assigned a random 16 character hexadecimal code as its identifier. Clicking on the “Results for submission: [hex]” link opens a page with the results. If you submit another workbook to run, the new results will append to this list. All analyses will be available until either the “Clear Page” button is pressed or the webpage is closed in your browser.



The screenshot shows a web interface for uploading and analyzing an Excel workbook. At the top, there is a text input field containing the filename "SISUS\_v0\_08-010\_Getting\_Started.xls" and a "Browse..." button to the right. Below the input field, the text "Current file: SISUS\_v0\_08-010\_Getting\_Started.xls" is displayed. To the right of the input field, the text "Upload SISUS Excel workbook for analysis" is shown. Below the input field and text, there is a blue "Analyse" button. A horizontal line separates the upload section from the results section. In the results section, the text "Results" is displayed. Below it, there is a blue link "Results for submission: 5341BF8D88F943EB". To the right of the link, the text "Parameter values:" is shown, followed by "filename = SISUS\_v0\_08-010\_Getting\_Started.xls". At the bottom of the results section, there is a blue "Clear Page" button.

Figure 22: Website Execute: Complete

## 4 Results

The results page is simply a list of files. At the bottom of the page are two links “Results only” and “Results and Data”. Clicking either of these will prepare a zip archive file that includes just the results, or the results and the Workbook, respectively. I recommend selecting “Results and Data” if you decide to retain the results.

Specific mixture results are created only when solutions exist.

### Results for submission: 5341BF8D88F943EB

[SISUS v0 08-010 Getting Started.xls](#)

[process info.txt](#)

[params 5341BF8D88F943EB.txt](#)

[SISUS GS v0 08 sisus inputs.txt](#)

[SISUS GS v0 08 plot convex hull Mixture 1 Isotope 1 Isotope 2.png](#)

⋮

Download this Results web page with the: [Results only](#) [Results and Data](#)

Figure 23: Website Results Page

The output requested in Output Settings of Worksheet 1 appears on the Results page. 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. process\_info.txt, text appearing in Process Log window copied to last file.
3. params\_[hex].txt, not important, just says what the filename was you submitted
4. 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.
5. 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.
6. 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.
7. 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.
8. [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.**

## 4.1 Process Log

Thought this is the last file, it should be checked first for the status of the execution. Figures 24–25 on pages 31–32 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 separately

**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 isotopic signatures 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 so
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 24: 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 25: Results, devel\_v01-07\_process\_info.txt (2 of 2)

## 4.2 Plots

All plots have four common properties. At the bottom, credit is given to SISUS: 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.

## 4.3 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).

### 4.3.1 One Mixture, pair of elements

Convex hull for one mixture and one pair of elements.

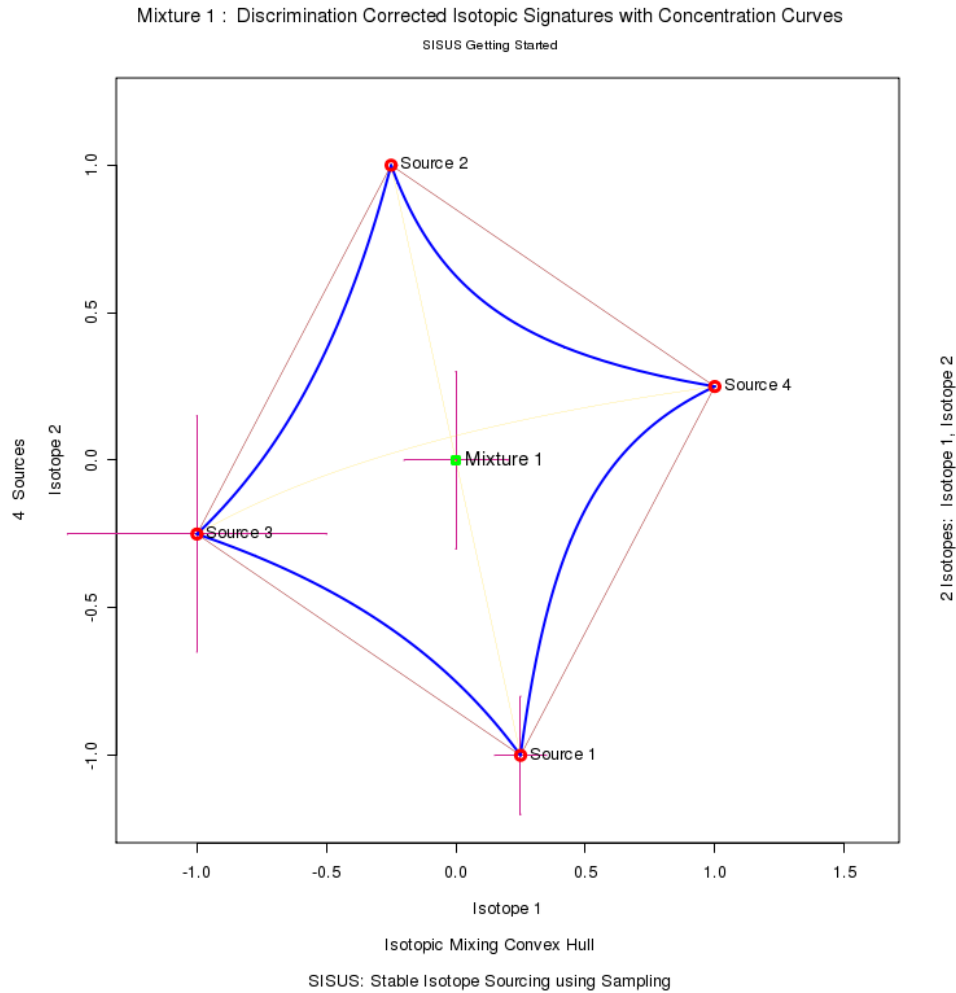


Figure 26: Convex Hull for Mixture 1, elements Isotope 1 and Isotope 2, file SISUS\_GS\_v0.08\_plot\_convex\_hull\_Mixture\_1\_Isotope\_1\_Isotope\_2

### 4.3.2 One Mixture, matrix of all element pairs

Convex hull matrix for one mixture and all pairs of elements.

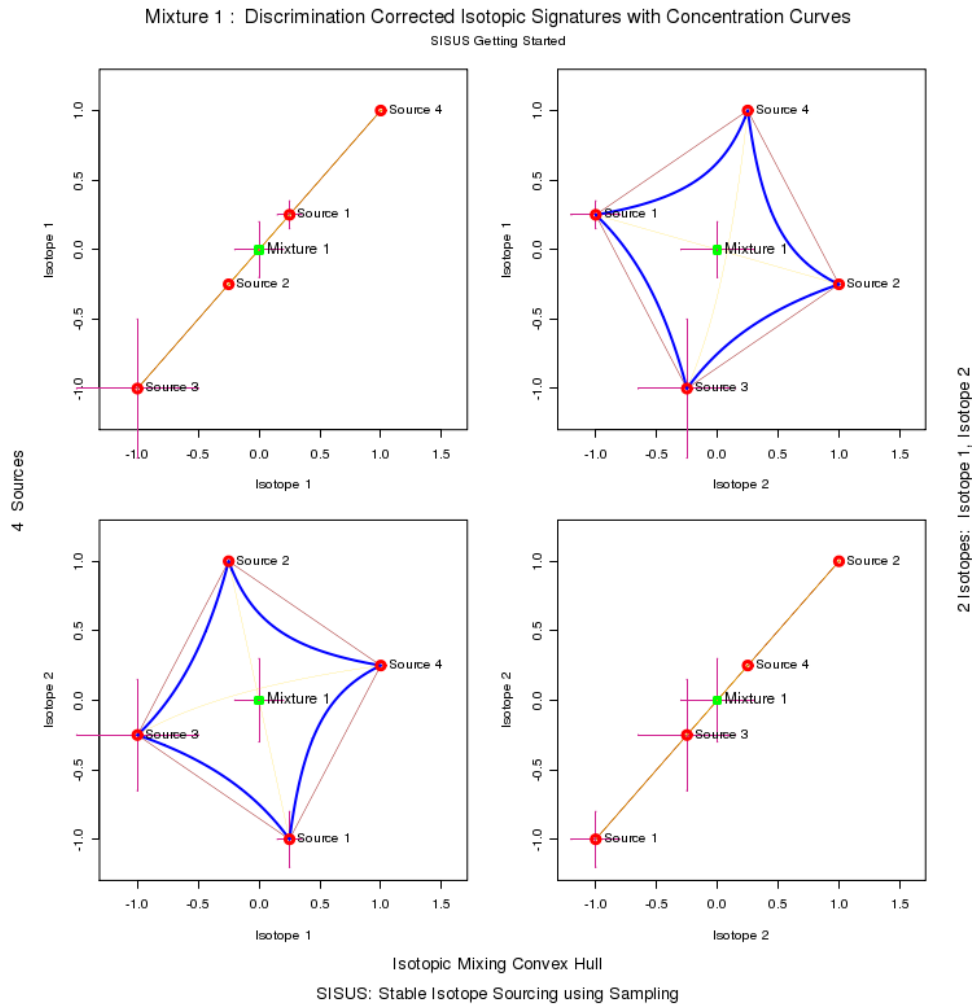


Figure 27: Convex Hull Matrix for Mixture 1, file SISUS\_GS\_v0.08\_plot\_convex\_hull\_matrix\_Mixture\_1

### 4.3.3 Mixture Group, pair of elements

Convex hull for mixture group and one pair of elements.

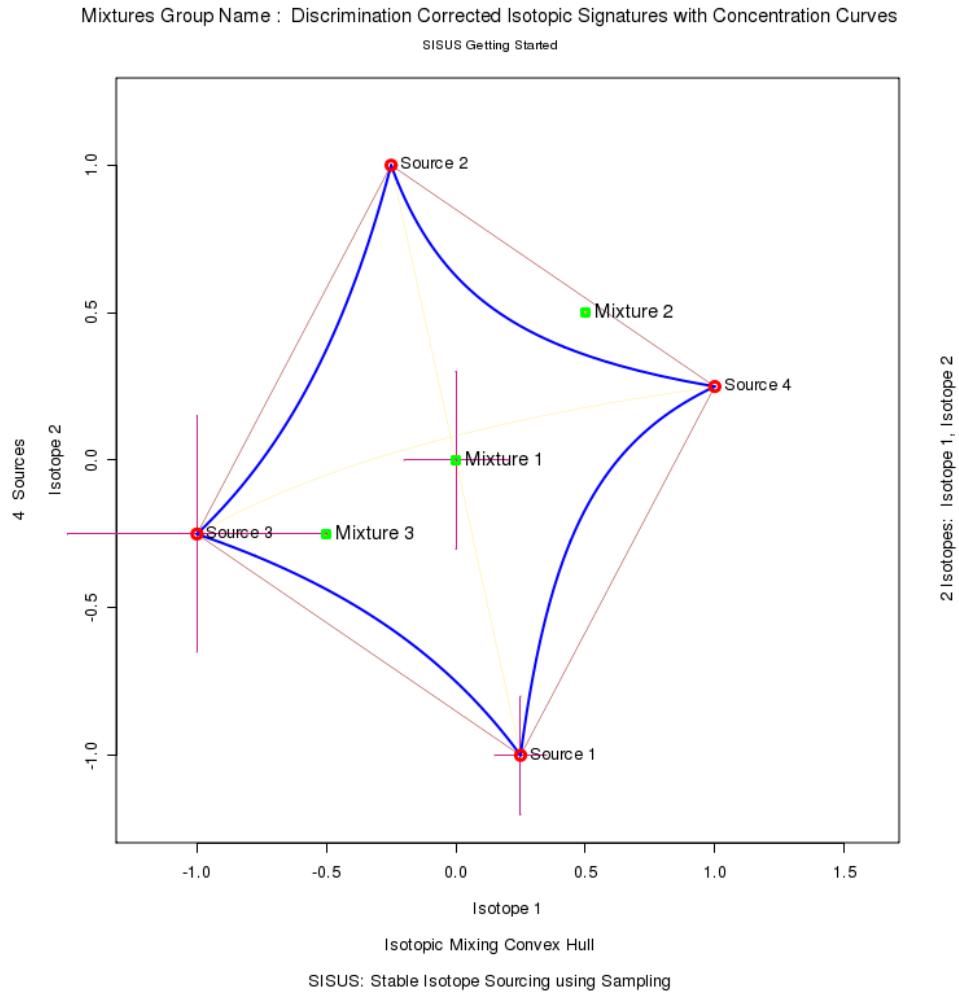


Figure 28: Convex Hull for Mixture Group, elements Isotope 1 and Isotope 2, file SISUS\_GS\_v0\_08\_plot\_convex\_hull\_Mixtures\_Group\_Name\_Isotope\_1\_Isotope\_2

### 4.3.4 Mixture Group, matrix of all element pairs

Convex hull matrix for mixture group and all pairs of elements.

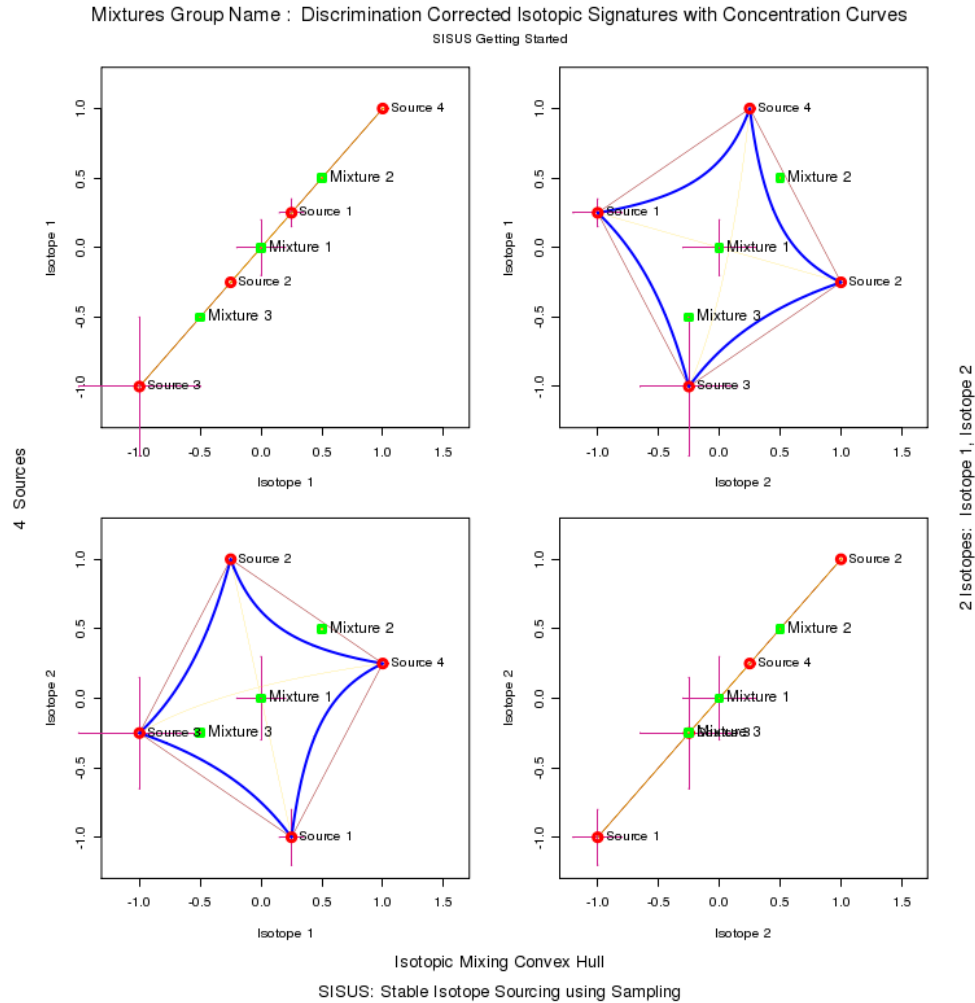


Figure 29: Convex Hull Matrix for Mixture Group, file SISUS\_GS\_v0.08\_plot\_convex\_hull\_matrix\_Mixtures\_Group\_Name

## 4.4 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 30 on page 38 is for Biomass proportions. When concentrations or assimilation efficiencies are specified, plots for the proportion of each element would also be created. Figure 31 on page 39 is for Isotope 1 proportions and Figure 32 on page 40 is for Isotope 2 proportions.

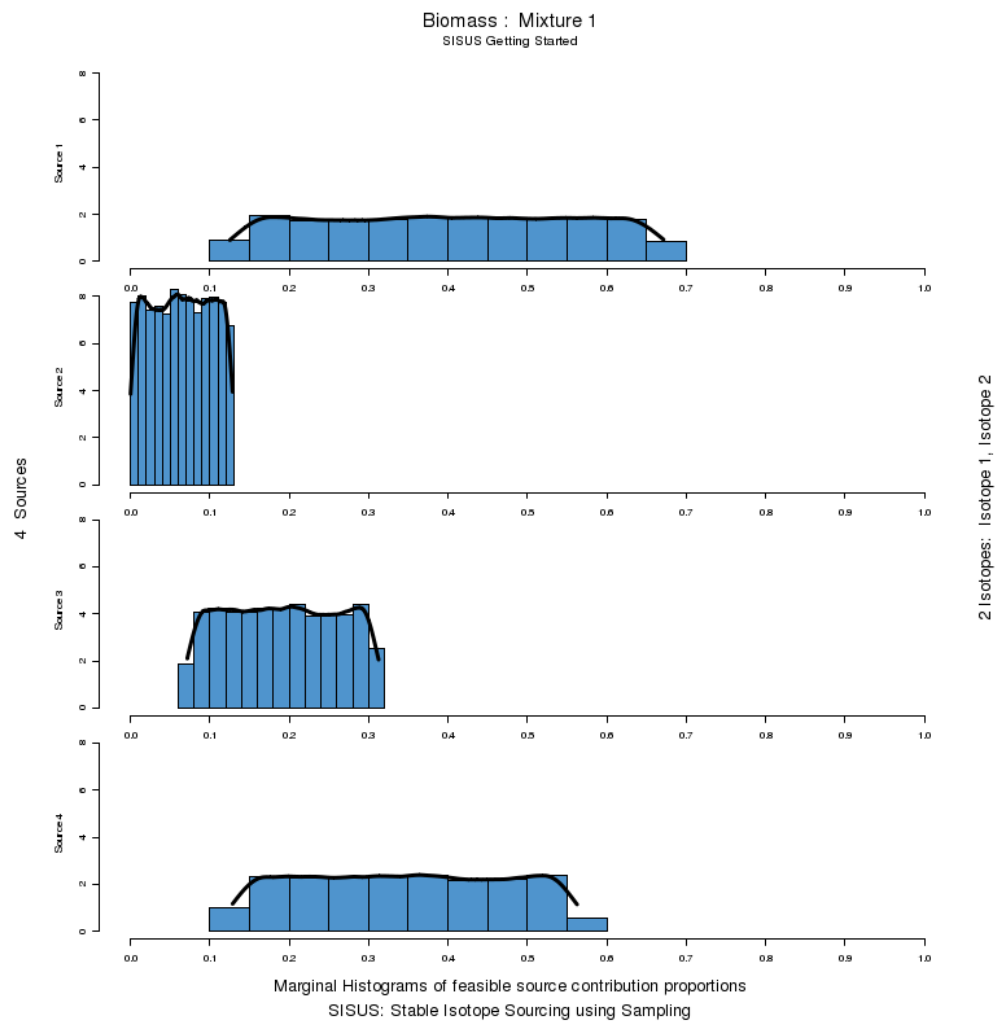


Figure 30: Marginal Histogram for Biomass for Mixture 1, file SISUS\_GS\_v0.08\_plot\_marginal\_hist\_unif\_sam\_Mixture\_1\_Biomass

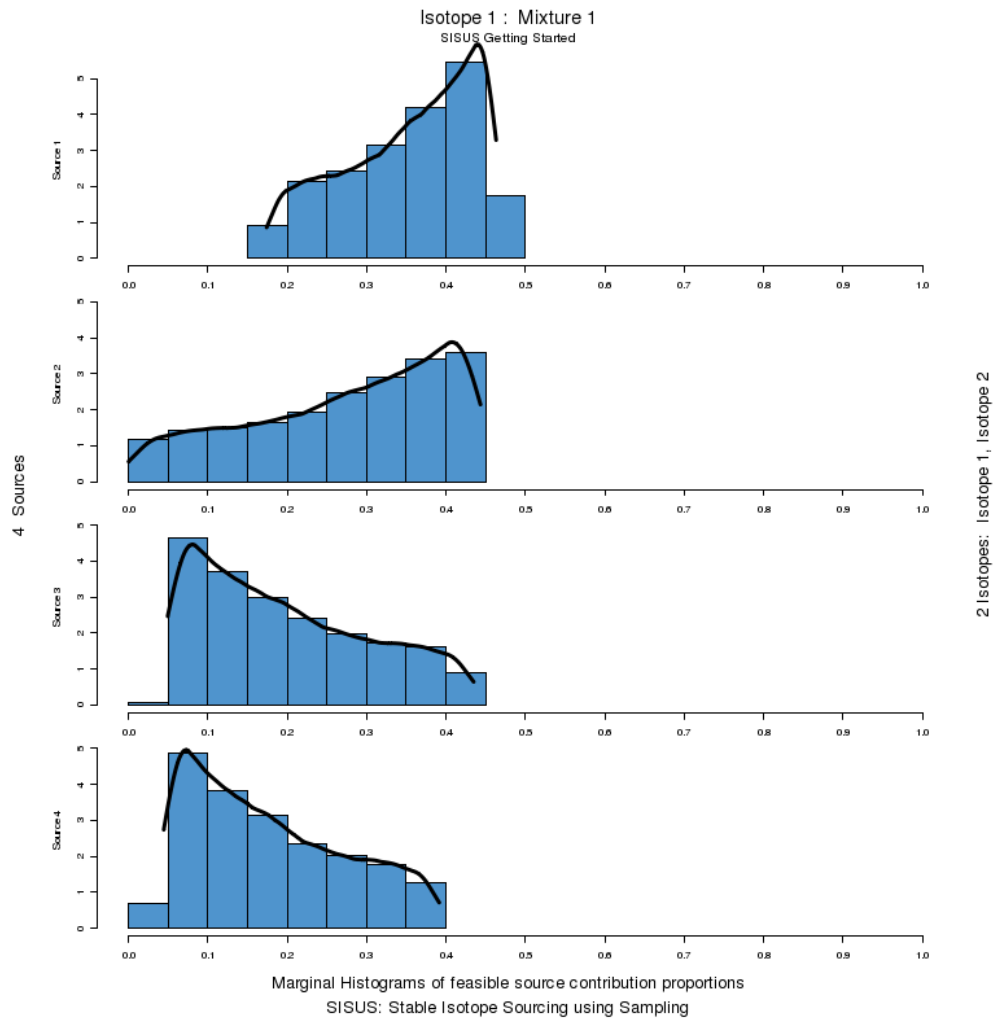


Figure 31: Marginal Histogram for Isotope 1 for Mixture 1, file SISUS\_GS\_v0.08\_plot\_marginal\_hist\_unif\_sam.Mixture\_1\_Isotope\_1

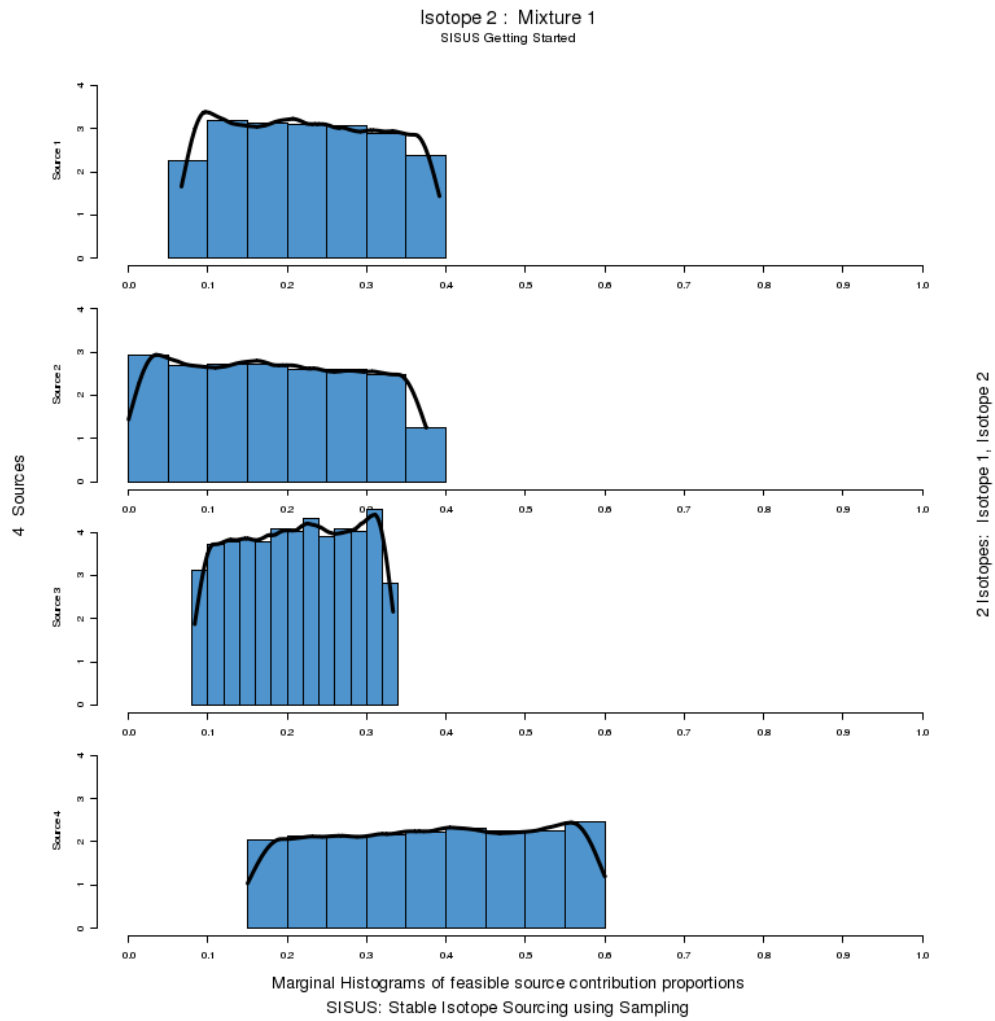


Figure 32: Marginal Histogram for Isotope 2 for Mixture 1, file SISUS\_GS\_v0.08\_plot\_marginal\_hist\_unif\_sam.Mixture\_1\_Isotope\_2

## 4.5 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 vertices 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 33 on page 42 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 34 on page 43 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 33: 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 34: Numerical Summaries, SISUS\_GS\_v0\_08\_sisus\_stats\_Mixture\_1.txt  
 (Dirichlet Resamples)



## 4.7 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 37 on page 46 shows the Biomass Uniform Samples for Mixture 1. Figure 38 on page 47 shows the Isotope 1 Uniform Samples for Mixture 1. Figure 39 on page 48 shows the Biomass Dirichlet Resamples for Mixture 1. Figure 40 on page 49 shows the Isotope 1 Dirichlet Resamples for Mixture 1.

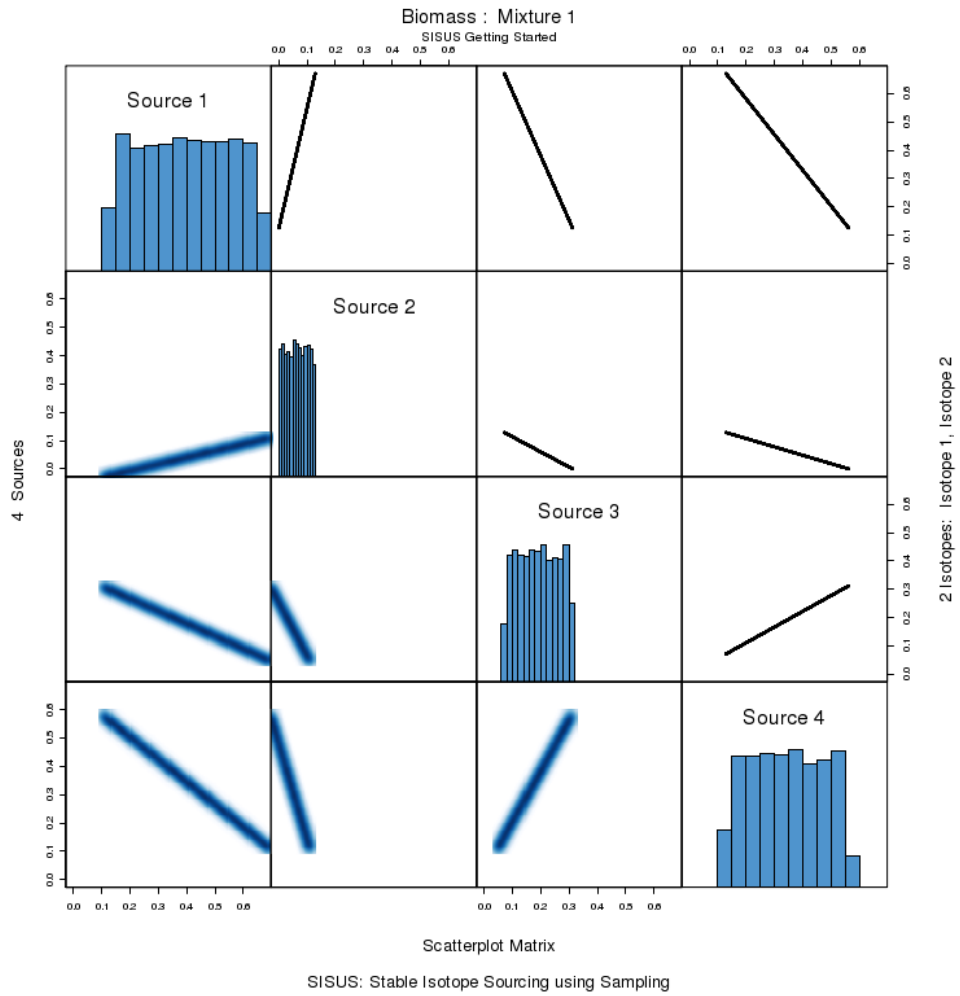


Figure 37: Scatterplot matrix, Uniform Samples, file SISUS\_GS\_v0.08\_plot\_scatterplot\_matrix\_unif\_sam\_Mixture\_1\_Biomass

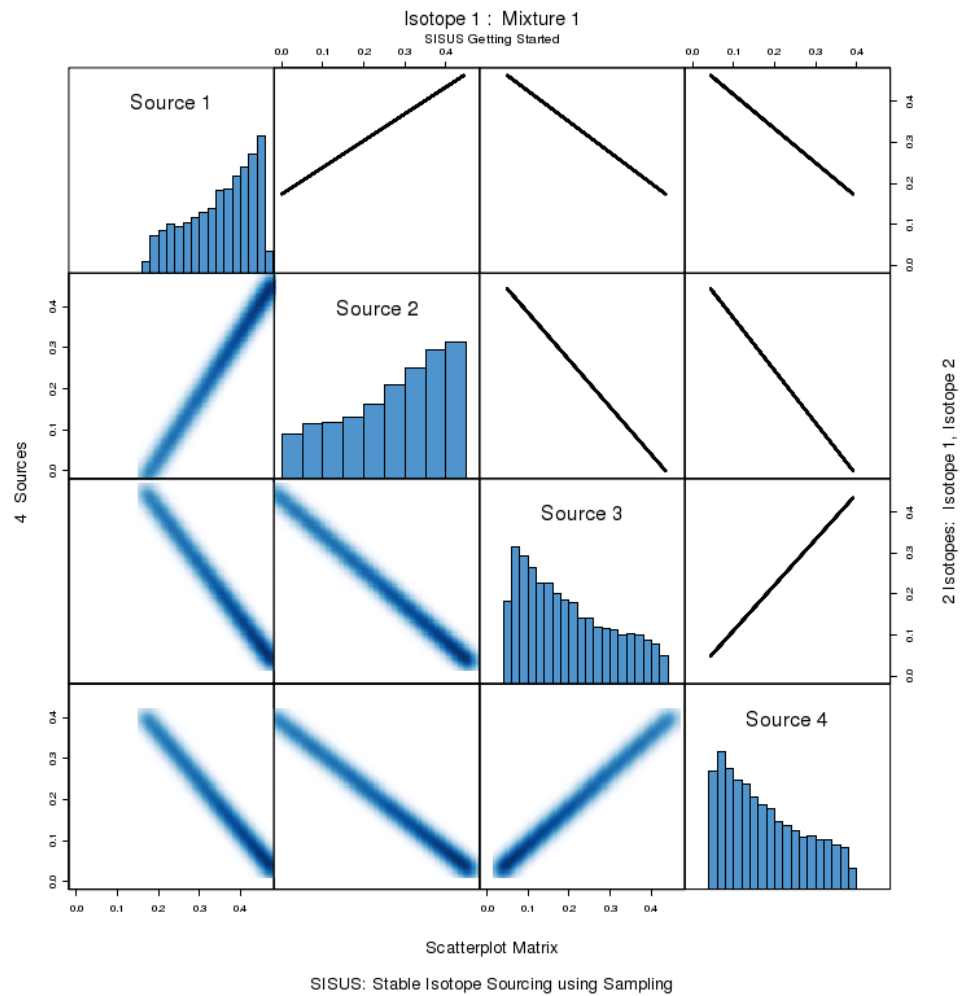


Figure 38: Scatterplot matrix, Uniform Samples, file  
SISUS\_GS\_v0.08\_plot\_scatterplot\_matrix\_unif.sam\_Mixture\_1\_Isotope\_1

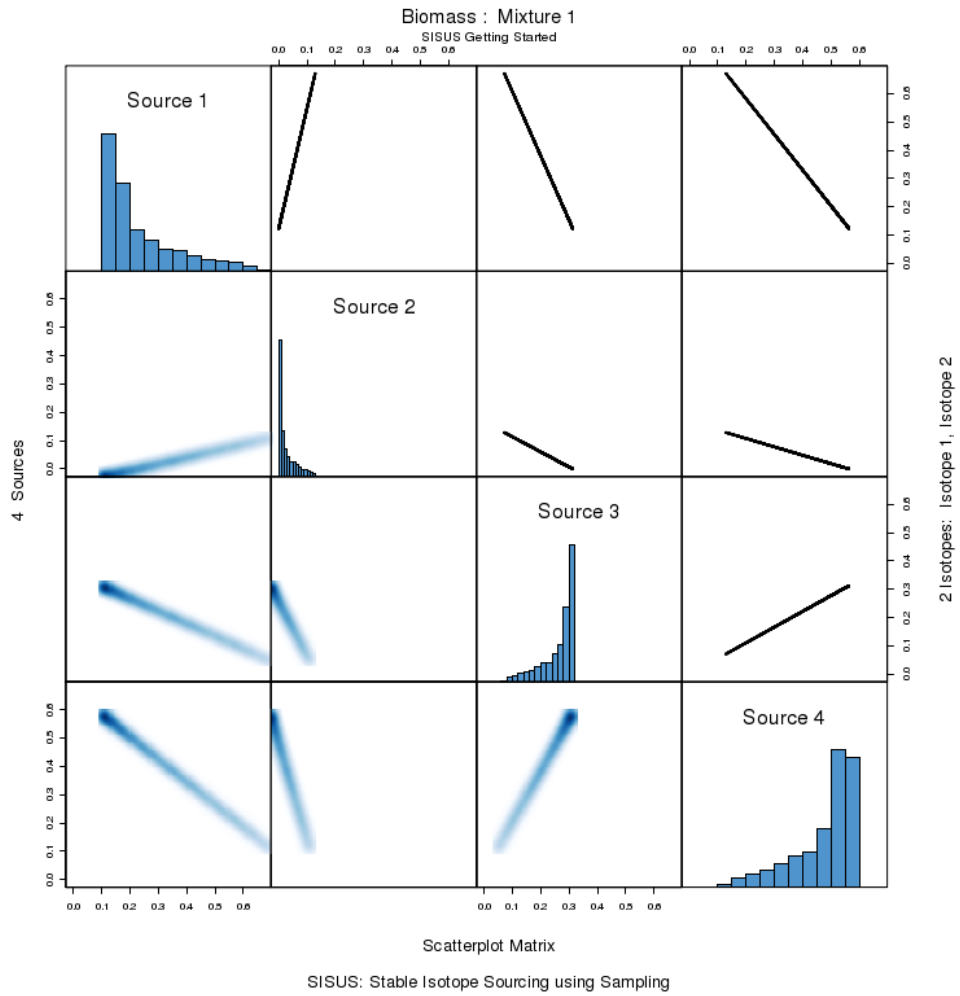


Figure 39: Scatterplot matrix, Dirichlet Resamples, file SISUS\_GS\_v0.08\_plot\_scatterplot\_matrix\_dir\_resam\_Mixture\_1\_Biomass

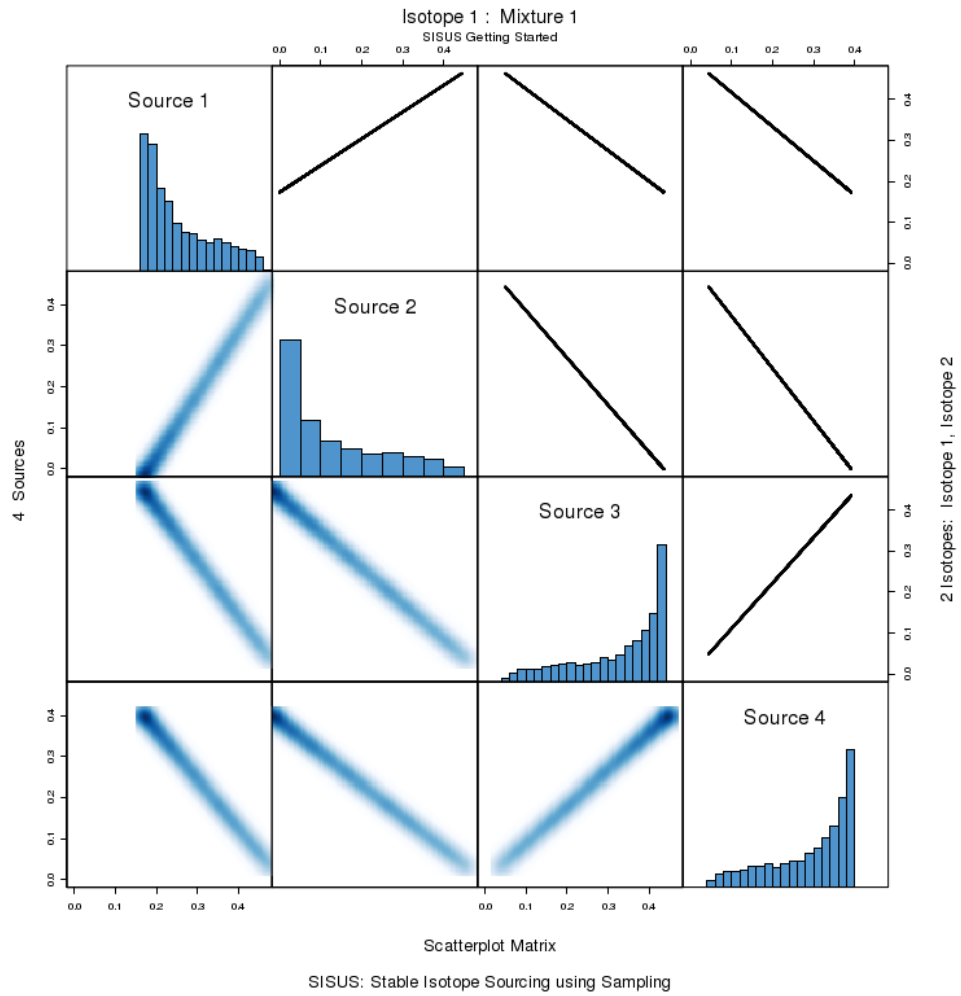


Figure 40: Scatterplot matrix, Dirichlet Resamples, file SISUS\_GS\_v0.08\_plot\_scatterplot\_matrix\_dir\_resam\_Mixture\_1\_Isotope\_1