Post-processing IsoSource results to incorporate additional non-isotopic constraints

The Phillips & Gregg (2003) paper described the IsoSource model, which was designed to give "the distribution of feasible source contributions based entirely on isotopic constraints when the number of sources precludes a unique solution. Given this information, it is possible to apply other constraints to further reduce the range of contributions from each source." This was discussed further and several examples were given. As pointed out in the paper, "One flexible way to incorporate such other factors is to give the entire range of solutions using only isotopic constraints, and then extract a subset of the output which also satisfies other non-isotopic constraints." Here we provide additional details about the mechanics of how this can be accomplished, and work through a detailed example.

IsoSource creates two output files in the designated output directory (the default is C:\Program Files\Iso_source\output). The file with the ".out" suffix gives the input data at the top of the file, followed by each individual solution that met the mass balance requirements. Each solution includes a fractional value (0-1) for the contribution of each of the sources. This file is in a comma-separated-value format, with commas separating each of the fields on each line. Each line contains 12 fields, but they may not all be used. Numeric values are simply shown as numbers, while alphanumeric strings are surrounded by quotes ("string"). Blank fields simply contain empty quotes (""). Each field is separated from the next by a comma. An example .out file and a line by line description are shown on the following two pages:

Example of .out file output

```
"Date: ","11/17/2003","Time: ","10:46:51 AM","","","","","","","",""
"Title: ","constraints ","","","","","","","","","",""
"Increment: ","1%","","","","","","","","","",""
"Tolerance:","0.2","","","","","","","","","",""
"Isotopes:","X","Y","","","","","","","","",""
"Mixtures:",6,6,"","","","","","","","",""
"Sources:","","","","","","","","","","",""
"A","0","10","","","","","","","","",""
"B","10","10","","","","","","","","",""
"C","10","0","","","","","","","","",""
"D","0","0","","","","","","","","",""
"","***************","***************","","","","","","","","",""
"FEASIBLE OUTPUT:","","","","","","","","","","",""
"A","B","C","D","","","","","","","",""
"--------------","--------------","--------------","--------------","","","","","","","",""
0,.58,0,.42,"","","","","","","",""
0,.58,.01,.41,"","","","","","","",""
0,.58,.02,.4,"","","","","","","",""
0,.58,.03,.39,"","","","","","","",""
0,.58,.04,.38,"","","","","","","",""“
```

the rest of the solutions follow here

input data

solution headers

solution data

Line by line description of example .out file

Line 1:	date and time stamp for IsoSource run
Line 2:	title of input data set
Line 3:	Increment value
Line 4:	Tolerance value
Line 5:	isotopic signature labels
Line 6:	mixture isotopic signatures
Line 7:	“Sources” title
Lines 8-11:	name of each source and its isotopic signatures
Line 12:	line of asterisks to separate input data above from solution data below
Line 13:	“Feasible output:” title
Line 14:	source name column headings
Line 15:	dashed line to separate column headings from solution data below
Lines 16-:	solutions (0-1 value for contribution of each source). The first such solution shows source contributions of A=0, B=0.58, C=0, D=0.42

NOTE: The number of lines naming the sources and giving their isotopic signatures (lines 8-11 in this example) will vary depending on the number of sources specified. This will determine on what line number the solution listing starts (line 16 in this example).

Using other software to impose additional constraints

Because there is such a variety of additional non-isotopic constraints that researchers may want to impose (see Phillips & Gregg 2003 for several examples), it was not possible to incorporate post-processing procedures in the IsoSource software that would be flexible enough to handle all these possibilities. However, the solution data in the .out file can readily be read into other software (e.g., Excel™, SAS™, S+™, Matlab™, Mathematica™, etc.) for further filtering of the results. The previous two pages outlined the record layout to facilitate input into other applications. In the following pages, we present a hypothetical example and show how the IsoSource output can be filtered to include other non-isotopic constraints.

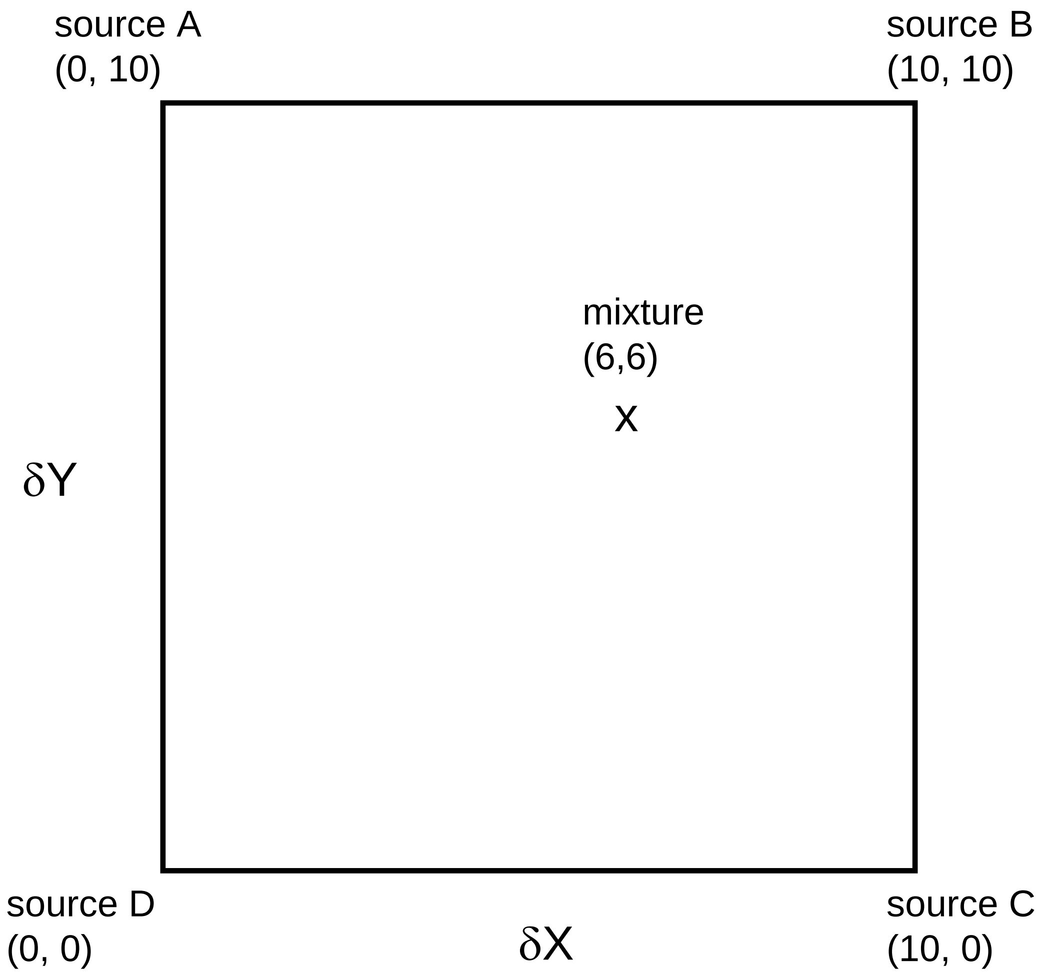
Our example is a dual isotope dietary study with 4 food sources. Suppose other ecological information was available about these food sources that indicated the contribution of source A to the assimilated diet must be greater than that of source B. This information might include relative abundance of food sources, ease of capture, stomach contents of the consumer, relative nutritional quality, etc. In any case, the additional constraint of A>B represents a condition necessary for ecological or physiological realism, based on information beyond isotopic signatures. Details of this example are shown as follows:

- page 5 – mixing diagram for 4 food sources and the consumer (mixture)
- page 2 – IsoSource .out file output
- page 6 – example SAS program to read .out file, graph the original solutions, impose additional constraint, compute statistics for and graph the constrained solutions
- page 7 – graphs of original IsoSource solutions
- page 8 – graphs of constrained solutions
- page 9 – summary of example, before and after post-processing for additional constraint

Hypothetical example to illustrate additional constraints:

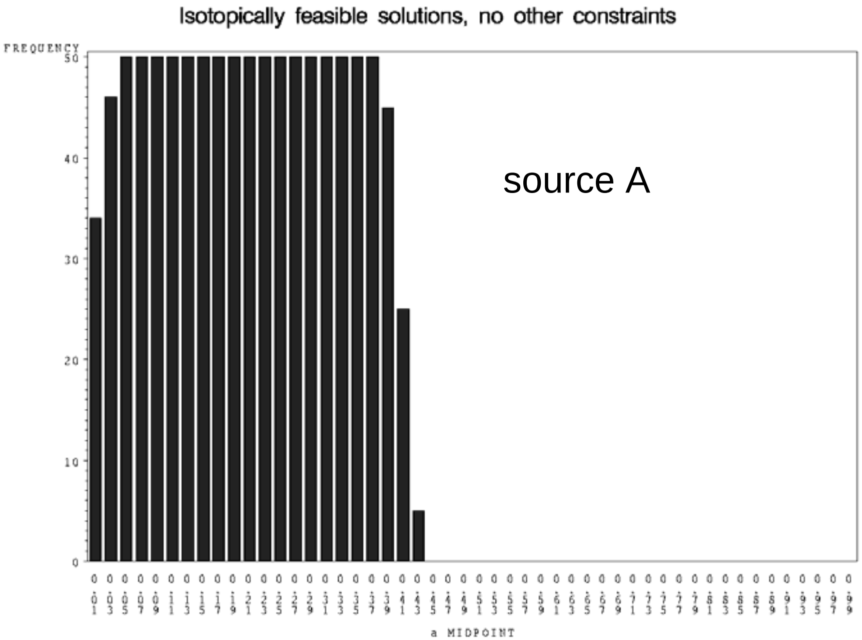
4 sources (A, B, C, D)

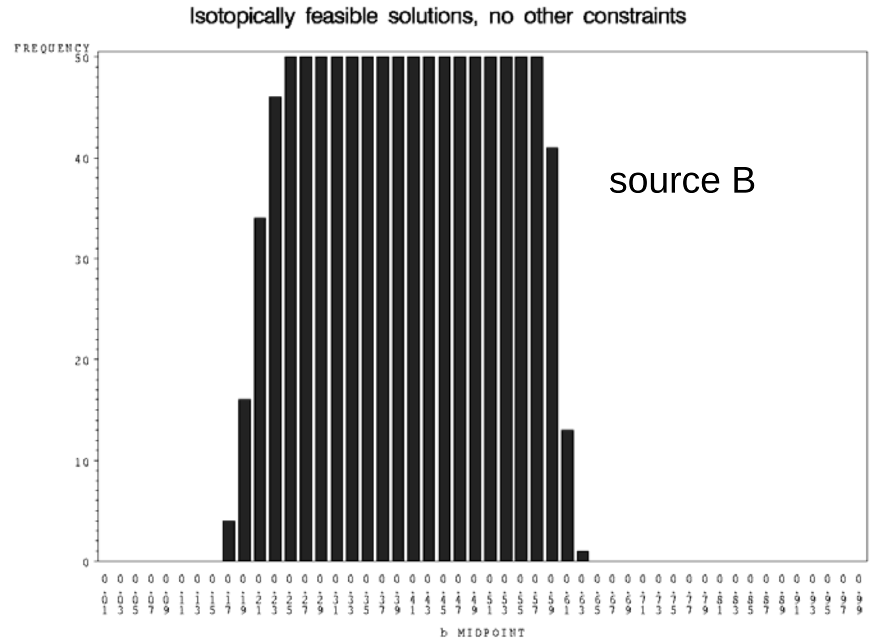
2 isotopic signatures (δX, δY)

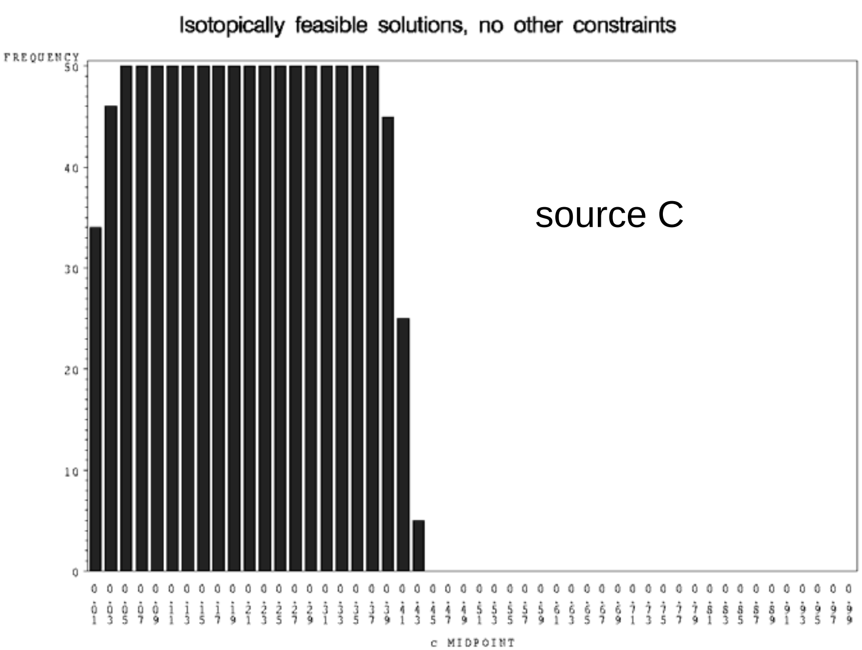


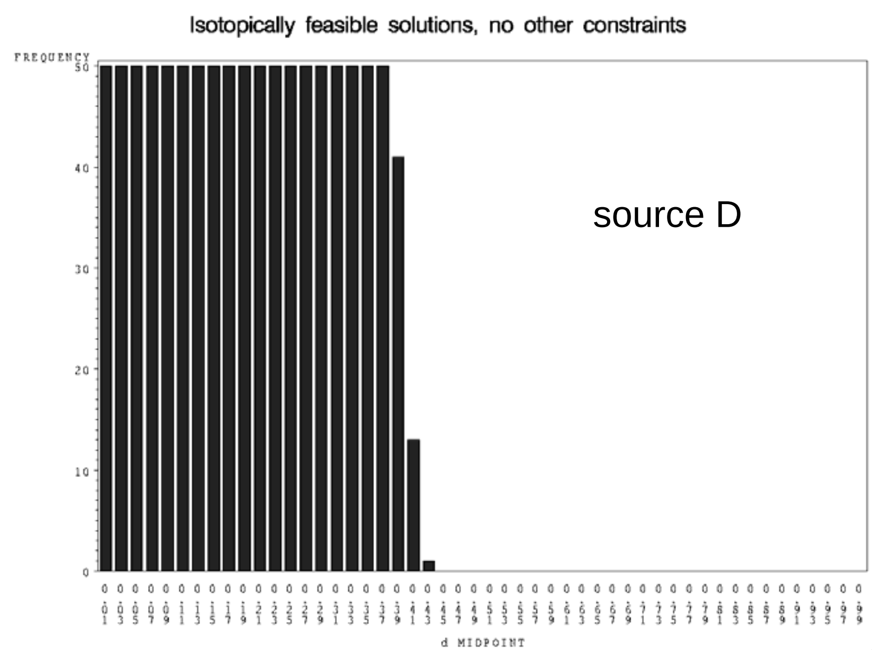
Example SAS program

```
*** READ IN ISOSOURCE SOLUTIONS ***;
data one;
   infile 'constraints.out' firstobs=16 dlm=',';
   input a b c d;
   title 'Isotopically feasible solutions, no other constraints';

*** PLOT HISTOGRAMS FOR ISOSOURCE SOLUTIONS ***;
proc gchart;
   vbar a b c d / midpoints=0.01 to 0.99 by 0.02;

*** IMPOSE ADDITIONAL CONSTRAINT THAT A>B ***;
data two;
   set one;
   if a>b;
   title 'Isotopically feasible solutions, other constraints: A>B';

*** DETERMINE N, MIN, AND MAX FOR CONSTRAINED SOLUTIONS ***;
proc means n min max;
   var a b c d;

*** PLOT HISTOGRAMS FOR CONSTRAINED SOLUTIONS ***;
proc gchart;
   vbar a b c d / midpoints=0.01 to 0.99 by 0.02;

run;
```

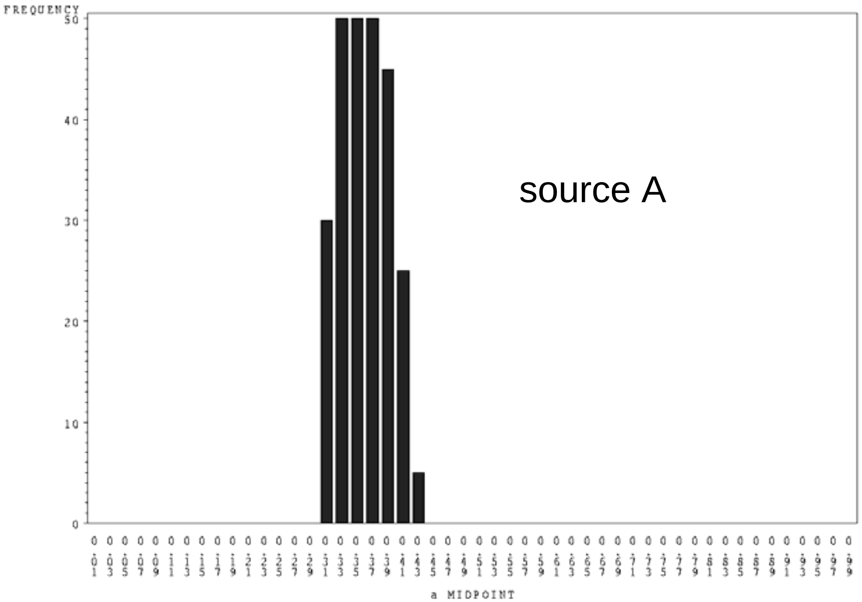

Isotopically feasible solutions, no other constraints
FREQUENCY
source A
a MIDPOINT


Isotopically feasible solutions, no other constraints
FREQUENCY
source B
b MIDPOINT

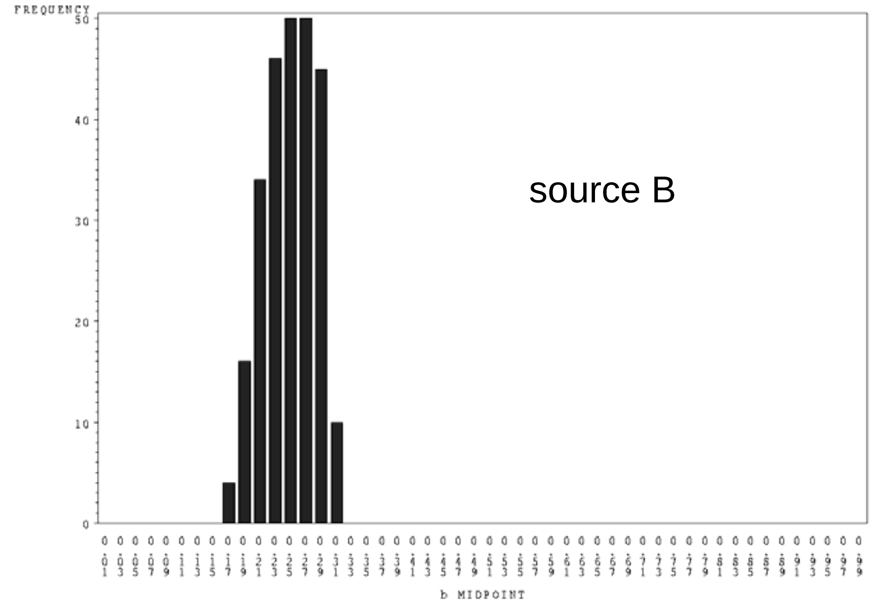

Isotopically feasible solutions, no other constraints
FREQUENCY
source C
c MIDPOINT


Isotopically feasible solutions, no other constraints
FREQUENCY
source D
d MIDPOINT

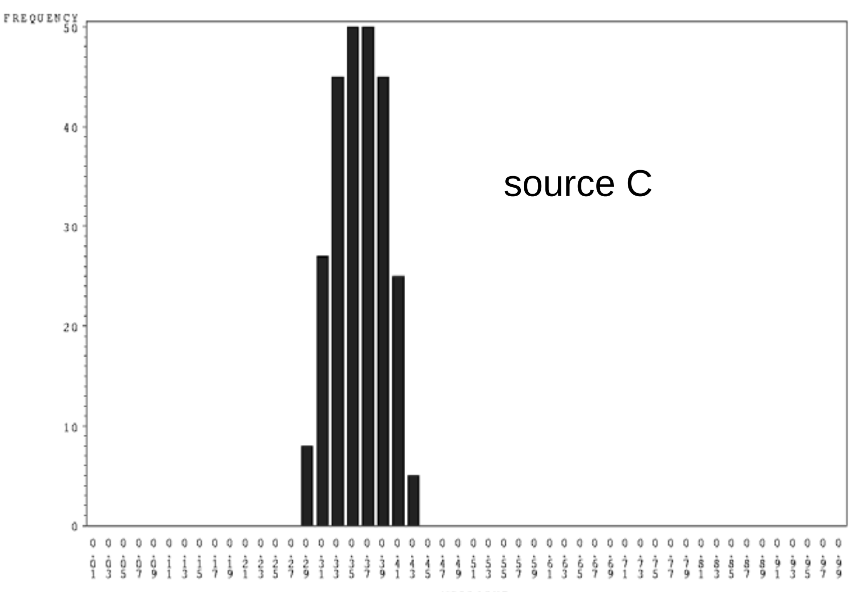
Isotopically feasible solutions, other constraints: A>B



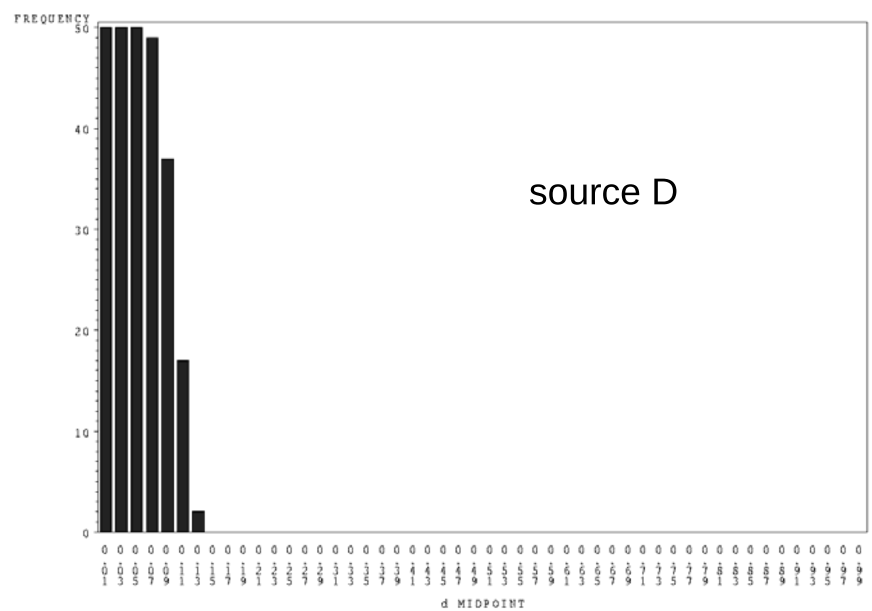
Isotopically feasible solutions, other constraints: A>B



Isotopically feasible solutions, other constraints: A>B



Isotopically feasible solutions, other constraints: A>B



Summary of example

- 4 sources (A, B, C, D)
- 2 isotopic signatures (δX, δY)
- IsoSource: increment=1%, tolerance=0.2

<u>no add'l constraints</u>

n=1005 solutions

A: 0 – 42%

B: 16 – 62%

C: 0 – 42%

D: 0 – 42%

constrain for A>B →

<u>constraint A>B</u>

n=255 solutions

A: 30 – 42%

B: 16 – 30%

C: 28 – 42%

D: 0 – 12%

Conclusion

In this example, the addition of one simple ecological constraint (A>B in the assimilated diet), reduced the ranges of possible source contributions to 1/3 or less of what they otherwise were. While a unique solution is still not possible, the combination of using IsoSource to determine the isotopically feasible solutions, along with further filtering of those results to incorporate other ecological constraints, provided informative results with reasonably narrow uncertainty bounds.

This example demonstrates how this process can be accomplished, as suggested in the Phillips & Gregg (2003) paper. In summary:

1) run IsoSource to determine solutions consistent with isotopic mass balance
2) read .out file into other software
3) impose additional constraints
4) report distribution of constrained solutions

As with unmodified IsoSource results, the following caveat (which is given in various forms in the software, on the web site, and in the paper) is applicable to any post-processing results:

NOTE - Each of the individual solutions represents a combination of source proportions which satisfies isotopic mass balance in the mixing model (*and other constraints if applied*). Descriptive statistics are provided simply as a way to characterize this entire distribution of feasible solutions. To avoid misrepresenting the results, users of this procedure should report the distribution of feasible solutions rather than focusing on a single value such as the mean.