READ ME First!

The attached zip file contains the source code needed to perform binary and ternary mixing inversions for ratio-ratio data, as well as several test files that may be used to ensure the code is functioning properly. The algorithms used in these codes are described in:

Sohn, R. A., A general inversion for end-member ratios in binary mixing systems, Geochem. Geophys. Geosyst, 6, Q11007, doi: 10.1029/2005GC000975, 2005.

and

Sohn, R. A., A method for inverting ratio-ratio data to estimate end-member compositions in mixing problems, Chemical Geology, 352, 63-69, doi: 10.1016/j.chemgeo.2013.06.002, 2013.

The source codes are written in Matlab. The source codes can either be placed in the working directory for a given dataset, or in specified directories that are automatically searched from Matlab command line input. Please see the Matlab help pages for more information, if necessary.

The inversion is performed by invoking the Hyperbolic_Mixing_3D.m script from the command line, and then providing some command line input regarding initial guesses for the mixing parameters and uncertainty estimation methods. The script then calls the necessary subroutines.

The code provides a variety of diagnostic plots, in addition to perspective views of the data and starting/final models. A histogram of normalized residuals is provided, along with histograms of the initial and final model parameters from the bootstrap replicates. If there is a significant offset between the initial and final histograms then it may be useful to run the inversion one more time using the posterior parameter estimates as the new starting model.

To test the code, you can use one of two synthetic datasets:

- binary mixing: Binary_test.dat
- ternary mixing: Ternary_test.dat

If you run the inverse for the binary test case using the following initial values:

X1=0.704
Y1=0.5129
X2=0.736
Y2=0.51208
c=0.4

then you should obtain the results shown in the file: Binary_test_results.txt

Note that the standard error estimates shown in this file were obtained using 500 bootstrap replicates. Because the bootstrap is a Monte Carlo type estimate, you may obtain slightly different error estimates even if you run the code with the same number of bootstrap replicates.

If you run the inverse for the ternary test case using the following initial values:

X1=0.702
Y1=0.51335
Z1=17.9
X2=.7055
Y2=0.5123
Z2=17.38
X3=0.7085
Y3=0.5125
Z3=19.1
Ka2b1=1
Kb1c2=2
Ka1c3=2
Ka1b3=1

then you should obtain the results shown in the file: Ternary_test_results.txt

As for the binary test case, the error estimates you obtain may be slightly different, but the parameter estimates should be identical.

If you have any problems please contact me: Rob Sohn, rsohn@whoi.edu

Good luck!