

Appendix A3.7: Input/Output For ML Estimation Of Mean And Variance

A3.7.1: Set-Up Requirements

To use the ML programs (Chung and Spirito, 1989), the geochemical data must be set up with an indicator variable following each value in the data file. If the data are not censored, a 0 follows the value. "Less than" and "greater than" signs are removed and the data value is followed by a "-1" or "+1" respectively. A BASIC program was used to convert the original geochemical files into the required format. The FORTRAN format statements that locate each element in the new file must be recorded and are used to tell the ML programs where a particular element can be found in a file. For example, the values below for sample, W and Au:

Sample	W (ppm)	Au (ppb)
6040	1130	<18
6041	35	<19
6044	<6	<13
6046	2370	32

would appear with indicator variables after them in the MLE file:

	1 1234 567890	1 5	2 0	2 5
6040	1130	0	18	-1
6041	35	0	19	-1
6044	6	-1	13	-1
6046	2370	0	32	0

Using the ruler bar above the file, the format statement for W is:
(4X,F8.0,I3)

A3.7.2: Output

The output from a run of the program to calculate mean and standard deviation follows:

```

USING THE NEWTONS SCORING METHOD
STEP 0    MEAN = -0.1309      S.D. = 0.6408
STEP 1    MEAN = -0.3811      S.D. = 0.7712
STEP 2    MEAN = -0.5415      S.D. = 0.9336
STEP 3    MEAN = -0.6470      S.D. = 1.0737
STEP 4    MEAN = -0.6966      S.D. = 1.1475
STEP 5    MEAN = -0.7059      S.D. = 1.1624
STEP 6    MEAN = -0.7062      S.D. = 1.1629
STEP 7    MEAN = -0.7062      S.D. = 1.1629

ML ESTIMATES FOR MEAN AND VARIANCE:  -0.70618      1.35242

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The ML estimators for sample mean and variance are calculated one element at time. The program is interactive and requests the user to specify input file name, sample size, format of the data and whether or not the log transformation of the data is required. It also requests the user to input the percentage of the detection limit to use as a replacement for any censored data in the file. As already noted, the choice of the starting point is arbitrary.

Step 0 is the starting point and the mean and standard deviation values are those obtained if the data set contains no censored data (i.e. if the censored values have been substituted with some percentage of their detection limit). The final step is the best possible estimate (i.e. no more improvements are made if more iterations are done). If the values are log-transformed, they cannot be applied to the data set directly (discussed in Section 4.3.6).