

Finding the Nearest Positive Definite Matrix for Input to Semi-automatic Variogram Fitting (varfit_lmc)

Arja Jewbali (arja.jewbali@riotinto.com)
Resource Estimation Geologist
Rio Tinto Iron Ore

In resource estimation work, variogram fitting is a routine process where geologist usually fit models independently to the experimental variograms of variables to be estimated. This process is time consuming and tedious when there are many variables per geological domain and many geological domains per deposit. Varfit_lmc, the semi-automatic variogram fitting routine developed at the Centre for Computational Geostatistics makes variogram fitting of multiple variables easier and faster by fitting a valid linear model of coregionalization (LMC) to all variables of interest. However, while the LMCs produced by prior versions of the program are valid, initial investigations found that the optimized nugget effects were often unrealistic, or a positive definite LMC matrix could often not be found when nuggets and sills were set by the user. This paper presents a method that determines the nearest positive definite matrix to a possibly non positive definite matrix input by the user in variogram fitting, and incorporates this method in the Varfit_lmc semi-automatic variogram fitting routine. The algorithm and its application are discussed and demonstrated using the Jura dataset.

Introduction

Varfit_lmc is a semi-automatic variogram fitting routine developed at the Centre for Computational Geostatistics (Larrondo, Neufeld and Deutsch, 2003 and Neufeld and Deutsch, 2004). Within varfit_lmc an initial model is gradually perturbed and with each perturbation the change in the objective function is noted. Only changes that minimize the objective function are allowed. Within the varfit_lmc routine the user has the option of fixing certain LMC (linear model of coregionalization) components such as the nugget, sills, structure types or the ranges of particular structures. When the nugget or sill components are fixed, the user needs to ensure that the initial matrices are positive definite. For a large number of variables, ensuring that the initial input matrices are positive definite can be tedious, requiring much trial and error. To solve this issue, a subroutine has been developed that finds the nearest positive definite matrix to a given non positive definite matrix was added to varfit_lmc.

Finding the nearest positive definite matrix is a matrix nearness problem where for a given matrix \mathbf{A} , the nearest member of a certain class of matrices needs to be found. Nearness (distance) is measured by some matrix norm. Higham (1989) describes different types of matrix nearness problems. In the approach described below the Frobenius norm will be used. If the distance norm is the Frobenius norm, then the nearest positive definite matrix to a given arbitrary matrix \mathbf{A} is relatively easy to determine and is given by the projection of \mathbf{A} on the positive definite cone of \mathbf{A} , which can be found by a spectral decomposition of \mathbf{A} (Boyd and Xiao, 2005). Calculation of the nearest positive definite matrix when nearness is measured by other norms than the Frobenius (i.e. 2-norm etc) is generally more complicated (Higham, 1989).

Methodology

An algorithm for determining the nearest positive definite matrix \mathbf{X}_F given an arbitrary $N \times N$ square symmetric matrix \mathbf{A} with real entries when nearness is measured using the Frobenius norm is given in Higham (1989) and proceeds as follows:

1. Determine the spectral decomposition of \mathbf{A} : $\mathbf{A} = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^T$ where \mathbf{Q} is a square $N \times N$ matrix which contains the eigenvectors of \mathbf{A} and $\mathbf{\Lambda}$ is a diagonal matrix with the diagonal entries being the corresponding eigenvalues λ_i of \mathbf{A} .
2. Next within $\mathbf{\Lambda}$ set each eigenvalue to 0 when $\lambda_i < 0$
3. Calculate $\mathbf{X}_F = \mathbf{Q}\mathbf{\Lambda}\mathbf{Q}^T$

The above described algorithm allows for deviation of the elements of matrix \mathbf{A} from the initial entries without constraint. Consider the following example where matrix \mathbf{A} is a matrix of nugget effect and cross nugget effects for 4 variables i.e. Cd, Co, Cr and Cu.

$$\mathbf{A} = \begin{bmatrix} 0.3000 & -0.2500 & -0.4000 & -0.5000 \\ -0.2500 & 0.2500 & 0.2400 & 0.1000 \\ -0.4000 & 0.2400 & 0.2800 & 0.5000 \\ -0.5000 & 0.1000 & 0.5000 & 0.2000 \end{bmatrix}$$

Matrix \mathbf{A} is not positive definite. Its eigenvalues are -0.3317; -0.1101; 0.1676 and 0.3042.

If the algorithm by Higham (1989) is used to calculate \mathbf{X}_F then the following matrix is obtained:

$$\mathbf{X}_F = \begin{bmatrix} 0.4128 & -0.2166 & -0.4057 & -0.3944 \\ -0.2166 & 0.2675 & 0.2083 & 0.1580 \\ -0.4057 & 0.2083 & 0.3990 & 0.3891 \\ -0.3944 & 0.1580 & 0.3891 & 0.3926 \end{bmatrix}$$

In matrix \mathbf{X}_F the diagonal elements (nuggets fitted to the auto variograms) have changed. The user might decide that a nugget of 0.39 for Cu is too high and would like to fix certain elements of matrix \mathbf{A} .

Incorporating equality constraints

To incorporate equality constraints the algorithm by Higham (1989) can be modified as follows:

- 1 Start by initializing $\Delta\mathbf{S}_0 = \mathbf{0}$ and $\mathbf{Y}_0 = \mathbf{A}$
For $k = 1, 2, \dots$
 $\mathbf{R}_k = \mathbf{Y}_{k-1} - \Delta\mathbf{S}_{k-1}$
- 2 Project \mathbf{R}_k on its positive definite cone to get \mathbf{X}_k i.e. steps 1, 2 and 3 from the algorithm by Higham (1989)
- 3 Calculate $\Delta\mathbf{S}_k = \mathbf{X}_k - \mathbf{R}_k$
- 4 Within \mathbf{X}_k set the matrix elements that need to remain fixed to their respective values and generate \mathbf{Y}_k .
End loop

This algorithm is known as the alternating projections method (Higham, 2002) and has been implemented in the varfit_lmc routine. In some instances the derived positive definite matrix might be very near to being negative definite and rounding errors might make the rounded matrix no longer positive definite. To generate a more robust positive definite matrix instead of setting the negative eigenvalues to zero,

they are set to a small positive number. This however, compromises on the nearness of the positive definite matrix to the initial input matrix. If nearness is important one can either place constraints on the trace of the matrix or reallocate the negative eigenvalues proportionally to the positive eigenvalues (Mueller, 2009).

If inequality constraints need to be placed on some or all of the matrix elements convex optimisation can be used to generate the nearest positive definite matrix (Boyd and Xiao, 2005). This was however, not implemented for varfit_lmc.

Positive definite partial sill matrices

Ensuring that the input matrix with the nugget effects for the LMC is positive definite, does not ensure that the matrices containing the partial sills for the LMC are also positive definite. Within varfit_lmc the user can either fix the nugget effects or the total sills. When the total sills are not fixed, the program calculates the total sills as the average of all experimental points at program initialisation. Similarly when the nugget effects are not fixed they are set to zero (starting value) at program initialisation. Depending on the number of structures specified by the user the starting values of the partial sills are set to the difference between the sill and the nugget divided by the number of structures (Larrondo, Neufeld and Deutsch, 2003).

When the user inputs a matrix of nugget effects, one way to ensure that the matrix of total sills is also positive definite is the following:

- 1 Make sure that the matrix of nugget effects \mathbf{C}_0 is positive definite. If it is not, use the algorithm described above to find the nearest positive definite matrix \mathbf{C}_0^P .
- 2 Calculate the difference matrix \mathbf{M} between the total sill \mathbf{C} and \mathbf{C}_0^P ($\mathbf{M} = \mathbf{C} - \mathbf{C}_0^P$). It does not matter if the total sill is user supplied or calculated by the program.
- 3 If the difference matrix \mathbf{M} is not positive definite, find its nearest positive definite matrix \mathbf{M}^P .
- 4 To get the positive definite total sill add the positive definite difference matrix and the positive definite \mathbf{C}_0 matrix ($\mathbf{M}^P + \mathbf{C}_0^P$)
- 5 The starting values of the partial sills can then be calculated by dividing the difference between the sill and the nugget effect (\mathbf{M}^P) by the number of structures and these partial sill matrices will be positive definite.

The workflow above is based on two properties of positive definite matrices:

- If two matrices \mathbf{A} and \mathbf{B} are positive definite, then their sum ($\mathbf{A} + \mathbf{B}$) is also positive definite.
- If \mathbf{A} is a positive definite matrix then $r\mathbf{A}$ is also positive definite for $r > 0$.

A multivariate example using the Jura data set

The Jura dataset contains seven variables sampled at 359 locations. A valid LMC needs to be fitted to all seven variables Cd, Co, Cr, Cu, Ni, Pb and Zn. For these seven variables (28 variograms in one direction) 56 variograms need to be fitted simultaneously in two directions. The variables have been standardized and the correlation matrix for the 7 standardized variables is given below in Table 1.

Table 1: Correlation matrix for the 7 standardized variables with strongly correlated variable highlighted

VARIABLE	Cd	Co	Cr	Cu	Ni	Pb	Zn
Cd	1	0.26	0.58	0.15	0.49	0.22	0.62
Co		1	0.48	0.19	0.74	0.16	0.44
Cr			1	0.21	0.71	0.26	0.61
Cu				1	0.22	0.82	0.66
Ni					1	0.27	0.59
Pb						1	0.67
Zn							1

As the table shows, the more strongly correlated variables are Co-Ni, Cr-Ni and Cu-Pb.

For input into varfit_lmc the following components have been fixed by the user:

- 1 The sills of the seven auto variograms are all set to unity, which is the expected sill of standardized variogram.
- 2 The sills of the cross variograms is set to the correlation respective coefficients listed in Table 1.
- 3 Following interpretation of the experimental auto variograms, the nugget effects of the auto variograms are set to the values listed in Table 2.
- 4 An isotropic model with two spherical structures was specified and the range of the second structure set to 1.3 km.

Table 2: Fixed nugget effects interpreted from experimental variograms

Variable	Nugget
Cd	0.25
Co	0.10
Cr	0.20
Cu	0.30
Ni	0.10
Pbi	0.35
Zn	0.10

After fitting the LMC with varfit_lmc, the matrix of total sills was checked as show in Table 3, which shows that the correlations between the variables listed in Table 1 are reproduced.

Table 3: Matrix of total sills for the fitted structures.

	Cd	Co	Cr	Cu	Ni	Pb	Zn
Cd	1	0.26	0.58	0.15	0.49	0.22	0.62
Co		1	0.48	0.19	0.74	0.16	0.44
Cr			1	0.21	0.71	0.26	0.61
Cu				1	0.22	0.82	0.66
Ni					1	0.27	0.59
Pb						1	0.67
Zn							1

The nugget effects fitted to the auto and cross variograms by varfit_lmc are listed in Table 4 below. The fixed nuggets for the auto variograms were fixed and remain the same as Table 2. If the user is not

satisfied with the values fitted to the cross variograms (the nuggets on the auto variograms were already fixed), there is the option to fix some or all of these and rerun varfit_lmc.

Table 4: Matrix of nugget effects for the fitted structures.

	Cd	Co	Cr	Cu	Ni	Pb	Zn
Cd	0.25	0.00	0.06	0.04	0.03	0.06	0.03
Co		0.10	0.03	0.00	0.01	0.00	0.00
Cr			0.20	0.02	0.04	0.03	0.03
Cu				0.30	0.00	0.17	0.09
Ni					0.10	0.00	0.00
Pb						0.35	0.08
Zn							0.10

Two spherical structures have been fitted:

- Structure 1 has a maximum range of 0.285 km and is isotropic.
- Structure 2 has a maximum range of 1.3 km and is isotropic.

The partial sill matrices for these two structures are shown in Table 5. These partial sills are all positive semi definite and the fitted LMC is thus valid.

Table 5: Matrix of partial sills for the fitted structures.

Structure 1							
	Cd	Co	Cr	Cu	Ni	Pb	Zn
Cd	0.579	0.000	0.394	0.098	0.171	0.112	0.437
Co		0.206	0.155	0.062	0.200	0.034	0.108
Cr			0.660	0.172	0.428	0.194	0.433
Cu				0.432	0.180	0.406	0.385
Ni					0.359	0.183	0.321
Pb						0.400	0.381
Zn							0.616
Structure 2							
	Cd	Co	Cr	Cu	Ni	Pb	Zn
Cd	0.171	0.259	0.127	0.009	0.291	0.045	0.152
Co		0.698	0.291	0.128	0.526	0.126	0.332
Cr			0.140	0.018	0.243	0.033	0.143
Cu				0.269	0.039	0.248	0.188
Ni					0.541	0.087	0.266
Pb						0.250	0.206
Zn							0.284

Given the noise in some of the cross variograms the program has provided a reasonable fit for the 7 elements. Plots of the experimental variograms against fitted models are shown in

Conclusion

Varfit_lmc has been shown to fit reasonable valid LMC models with user input of nugget/sill matrices, ranges and structure types. The program can handle a large number of variables and is quick to use and provides a more holistic approach to independent modeling of multiple variables in resource estimation.

The initial nugget and sill matrices input by the user do not have to be positive definite since the program determines the nearest positive definite matrix when the input matrices are not positive definite.

References

- Boyd, S. and Xiao, L., 2005, Least-squares covariance matrix adjustment: *SIAM Journal on Matrix Analysis and Applications*, v 27, no 2, p. 532-546.
- Higham, N., 1989, *Matrix Nearness Problems and Applications*: M. J. C. Gover and S. Barnett, editors, *Applications of Matrix Theory*: Oxford University Press, p. 1-27.
- Higham, N., 2002, Computing the Nearest Correlation Matrix-A Problem from Finance: *IMA Journal of Numerical. Analysis*, v 22, no3, p. 329-343.
- Larrondo, P.F., Neufeld, C., and Deutsch, C.V., 2005, *Varfit: A program for semi-automatic variogram modeling*: Fifth annual report of the Centre for Computational Geostatistics.
- Mueller, U., 2009, Personal communication.
- Neufeld, C., and Deutsch, C.V., 2004, *Developments in semi-automatic variogram fitting*: Sixth annual report of the Centre for Computational Geostatistics.

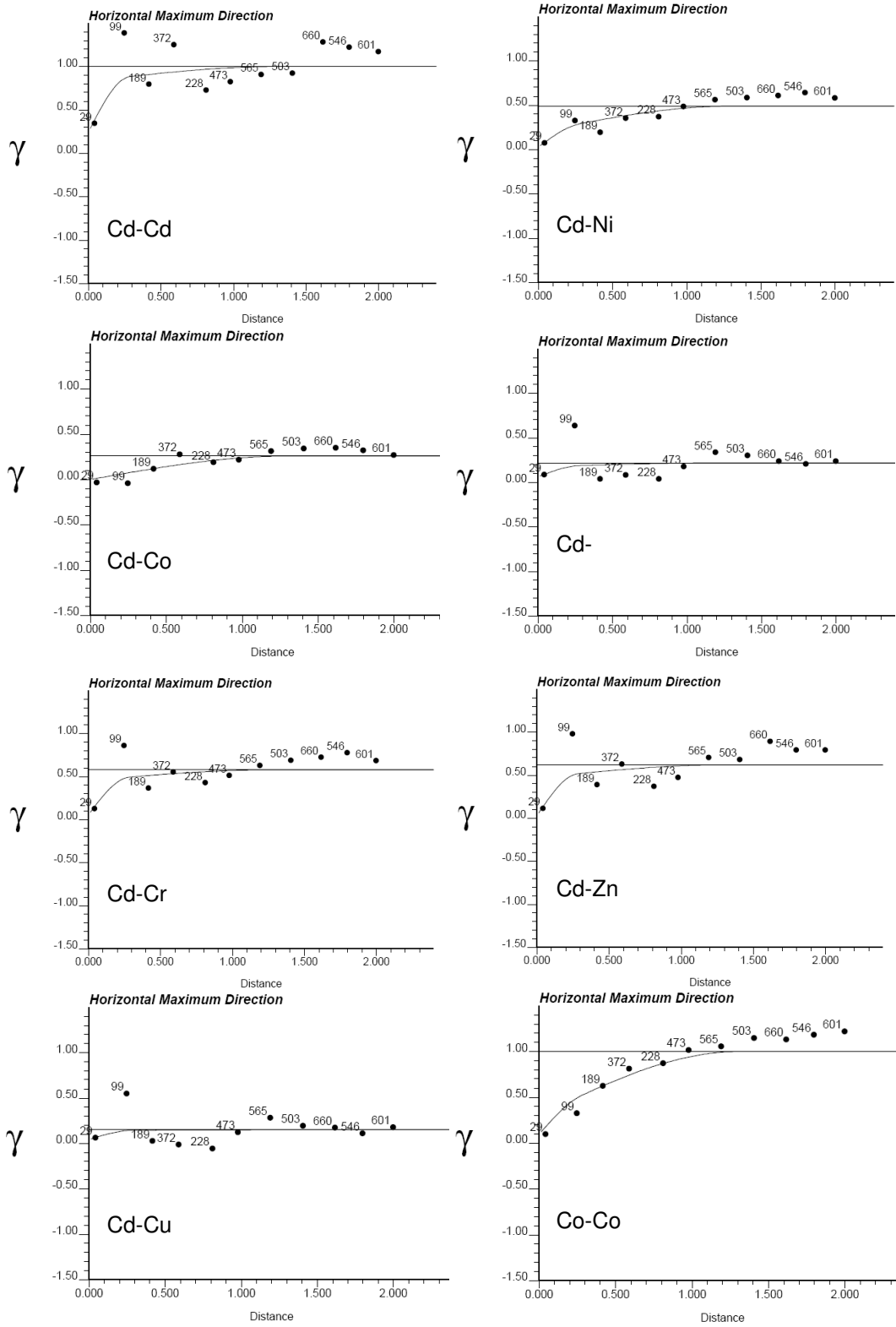


Figure 1. Fitted auto and cross variograms for Cd and Co

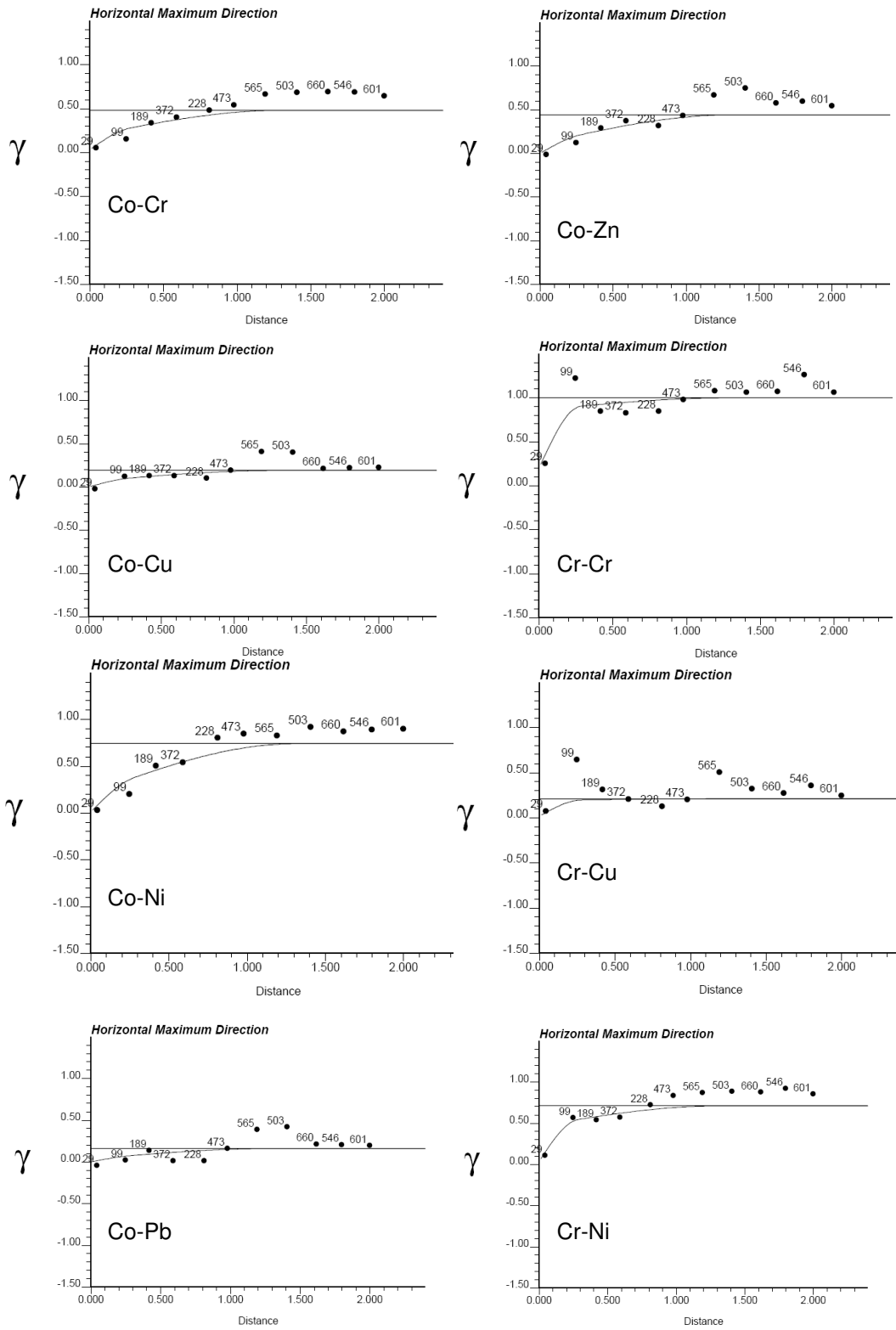


Figure 2. Fitted auto and cross variograms for Co and Cr

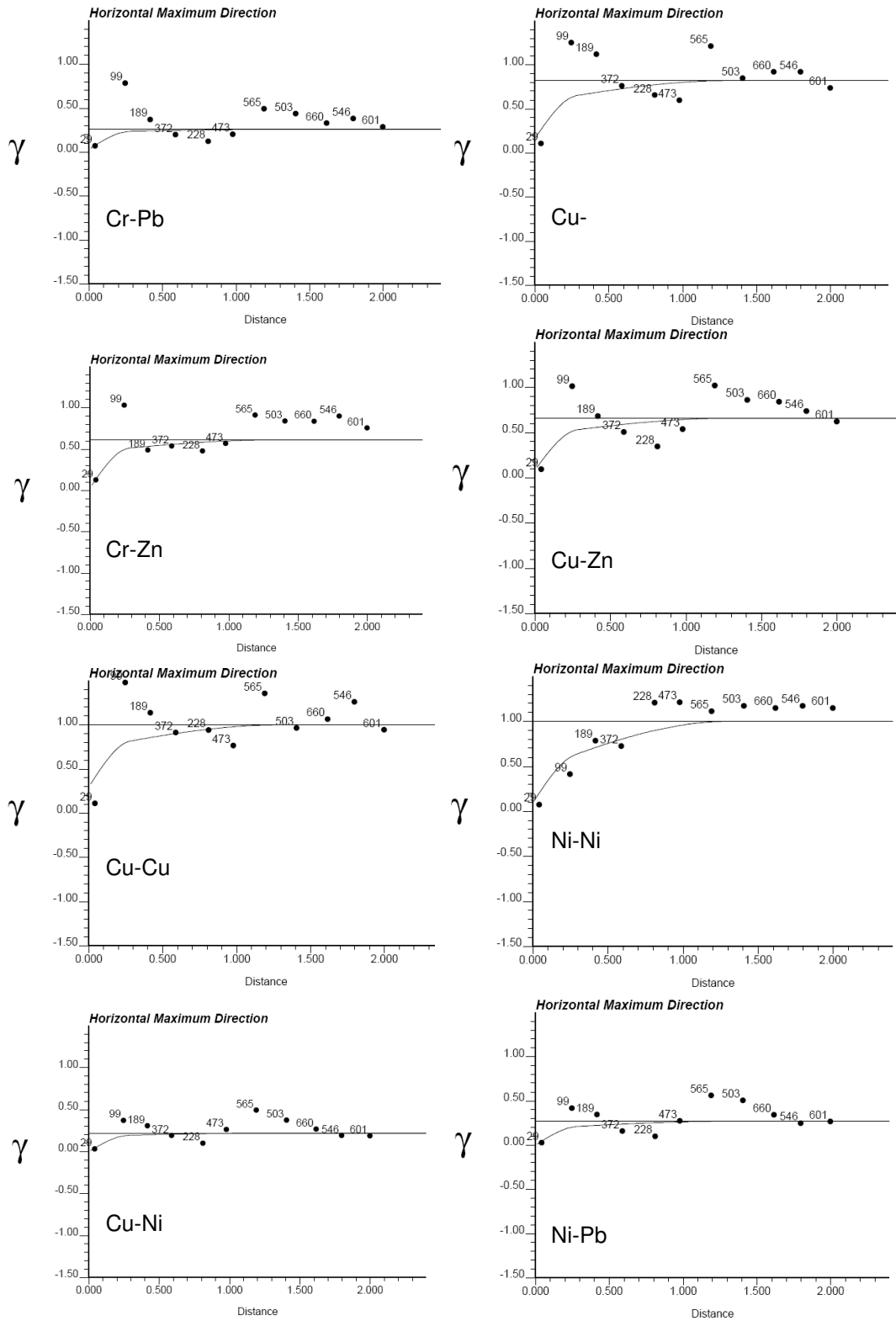


Figure 3. Fitted auto and cross variograms for Cr, Cu and Ni

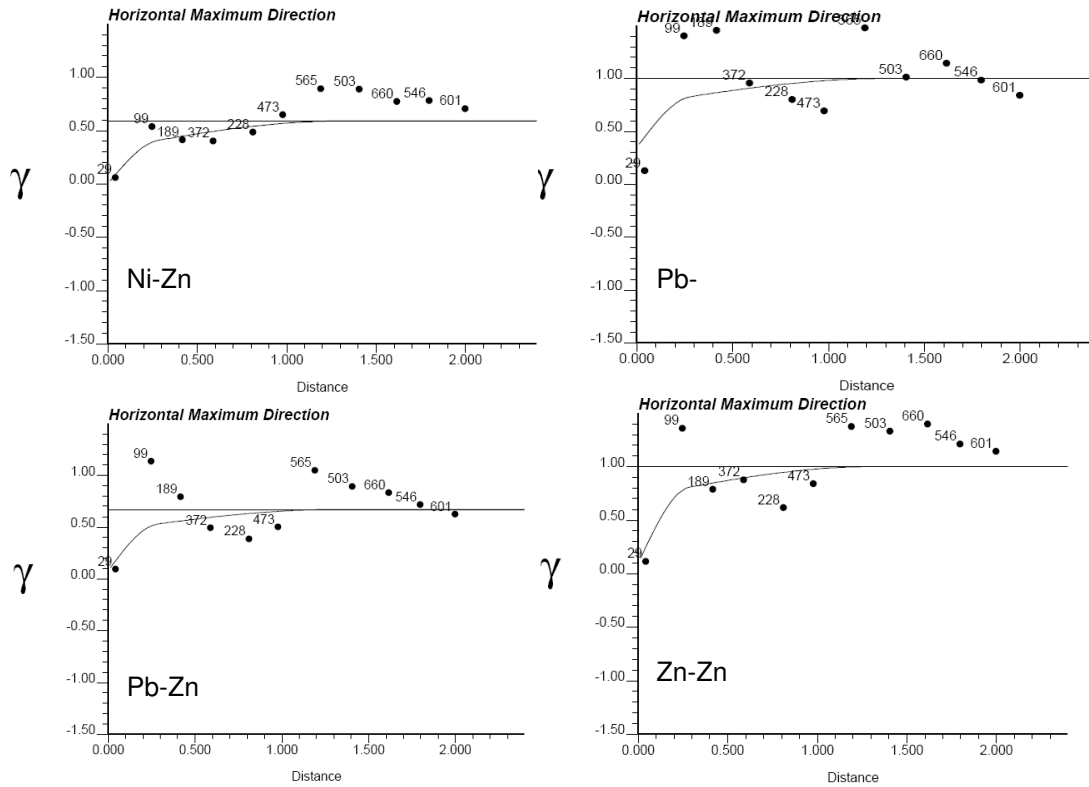


Figure 4. Fitted auto and cross variograms for Ni, Pb and Zn