Grain variogram calculation code – by Abhishek Bihani

This Python 3 code attempts to examine if there are spatial correlations between the different spherical grains in a bidisperse (two-sized) grain pack (Figure 1), by constructing variograms for measuring the spatial distribution of grain volumes and the inter-granular distances. Investigation of correlated spatial heterogeneity is important for reservoir characterization in the petroleum industry. The inputs for the code are the co-ordinates of all the spherical grains, their diameters (refer .csv file) and the length of grain pack, and the output is a variogram.

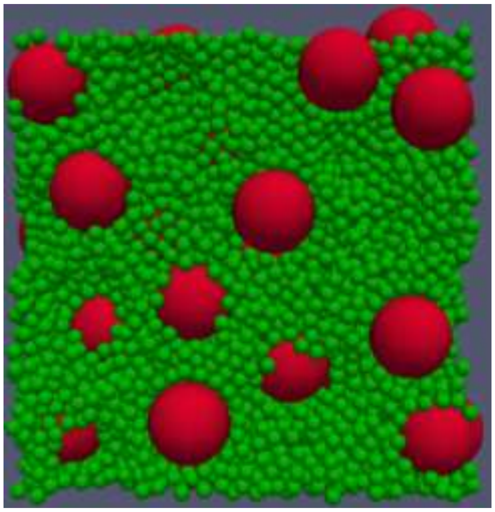

Figure 1- Code input example: Grain pack of two different sized spheres

Theory:

The variogram (γ) for the lag distance H is defined as,

$$\gamma(H) = \frac{1}{2N(H)} \sum_{N(H)} [z(u) - z(u+H)]^2, \tag{1}$$

where N(H) is the number of possible pairs of data for lag H, and z(u) is the stationary function corresponding to the grain volume (Pyrcz and Deutsch, 2014). The lag distance is the distance between data pairs for which the variogram is calculated. It is selected in order to get the maximum data in each lag and usually coincides with the data spacing. The minimum lag distance was considered 0.2 for all simulations as it is the minimum spacing between the grains. The stationary function was grain volume (V) calculated by equation (2) where r is grain radius, is the scalar variable associated with a location u and was used to calculate the variogram,

$$V = \frac{4}{3}\pi r^3. \tag{2}$$

The variograms were normalized with respect to the variance (*var*). The variance was calculated using Python's library 'NumPy' and is given by equation (3), where n is the total number of grains and z(avg) is the average grain volume,

$$var = \frac{1}{n}\sum[z(u) - z(avg)]^2. \tag{3}$$

Example:

A sample input to test the code has been provided (test1.csv). It is a grain pack of 2663 spheres, out of which 5 are large (r=0.5 unit) and 2658 are small (r=0.1 unit). The length of the grain-pack is 3 in all directions.

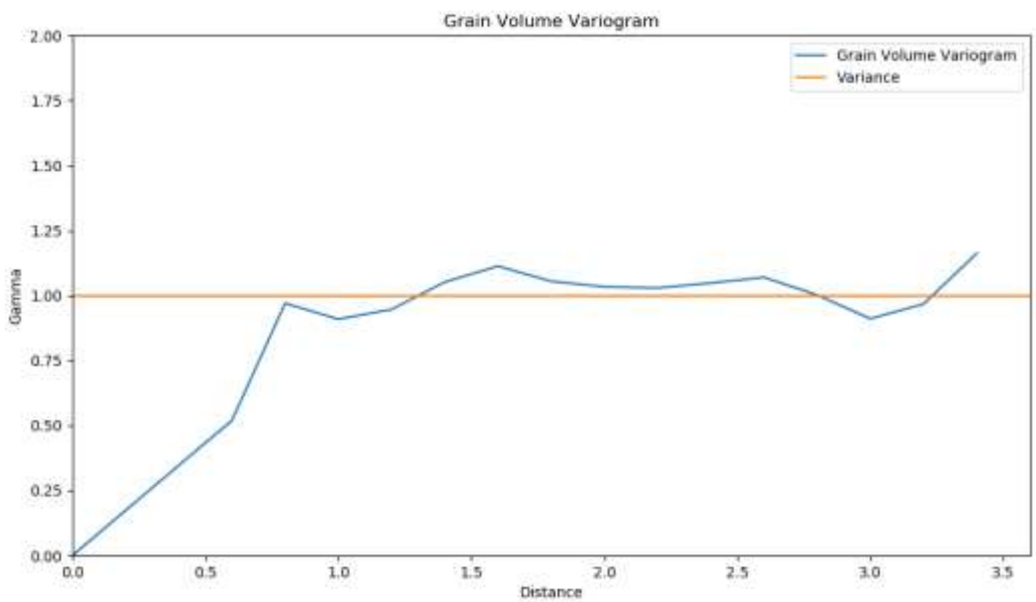

Figure 2- Expected code output: Variogram of the grain pack

An example of the expected output of the code is given in Figure (2). The blue line represents the variogram and the red line represents the variance (sill) with a constant value of one. When the variogram is lower than the variance, there are positive correlations between the different grains and when the variogram is higher than the variance, there are negative correlations between the grains. Figure 2 shows that while there is a positive correlation at low distances, due to smaller grains in close proximity with each other, the variogram begins approaching the variance value which signifies random distribution. At distances near the sample length, due to fewer number of data points, some deviation from variance may be observed.

References:

Pyrcz, M. J., & Deutsch, C. V. (2014). Geostatistical reservoir modeling. Oxford university press.