Lab 2. Variograms and their estimation

Math 586. Due October 10, 2017

Simulation

Here, the properties of different variogram models are illustrated through examples and simulation. For the source Matlab code and data files, see www.nmt.edu/~olegm/586/Lab2

- “White noise” or “pure nugget” random field. This is just a group of independent random variables, with the same mean 0 and variance $\sigma^2$. Corresponds to the variogram

$$\gamma(x) = \sigma^2, \quad x > 0$$

To simulate white noise, just use a random number generator. The output, by default, will consist of independent realizations:

```matlab
n = 1000;
sigma = 5;
wn = normrnd(0,sigma,n,1);
figure(1); plot(wn)
figure(2); plot(xcov(wn))
```

(We will start with 1-d simulations, for which the autocovariance plot is still valid; the variogram is the “upside-down” covariance.) Any other model with a nugget of a given size can be generated by adding white noise to the random field without nugget.

- **Brownian motion.** This can be thought of as cumulative sums of a white noise sequence (see the discrete example in Lecture 8, p. 1). An efficient realization looks like this:

```matlab
bm = cumsum(wn);
figure(1); plot(bm)
figure(2); plot(xcov(bm))
```
Brownian motion has a linear variogram with no sill, therefore it’s not stationary! However, like most IRF-0, it can be reduced to a stationary field (here, white noise) by differencing.

- **Other variogram models.** We will cover the principles of simulation later, in greater detail. For now, we will simulate from popular models covered by the Matlab program `randomfield.m` by Olaf Arie Cirpka, see
  
  http://m2matlabdb.ma.tum.de/download.jsp?MC_ID=5&MP_ID=31

  Try to compare Gaussian and exponential models, also try different variances for x and y (anisotropy) and different azimuth angles.

### Empirical Variograms

Here, we are using the Matlab program `variogram.m` created by Armando Zaupa Remacre, see

  http://www.mathworks.com/matlabcentral/fileexchange/4223

As an example, consider the CaMg data.

```matlab
data = load('camg1.csv');  \ % CaMg data, variable = ca020
V = data(:,5);  \ x = data(:,1);  \ y = data(:,2);
n = length(V);
x = x - mean(x);
y = y - mean(y);  \ % centering, otherwise the quadratic fit will be wrong
plot3(x,y,V,'.');
```

The plot reveals the presence of a quadratic trend. Therefore, we would first try to eliminate the trend (omitted here, see the online Matlab code)\(^1\) and then fit the variogram to the residuals.

```matlab
g = variogram(x, y, resid,0);
```

Choose the bins by yourselves, but they should not span more than half of the minimum spatial dimension.

### Variogram fitting

We can try different models and see which one fits better. Choosing “the right” model is not easy! Some experience and knowledge of underlying physics would help. Also, some formal criteria are available.

We will apply the *weighted least-squares* technique. That is, the best fit is the one that minimizes the squared distance between the empirical and the

\(^1\)Note that the centering (subtracting the mean) is done to ensure numerical stability.
modeled variogram. Each point of the empirical variogram will be weighted by the number of pairs it represents, times the inverse square of the fitted variogram value $\gamma$ (so that the smaller values of $\gamma$, closer to the origin, receive a higher weight).

The optimization is non-linear, so we’ll use a built-in Matlab routine \texttt{fminsearch}. In the example code, we fit Gaussian model

$$
\gamma(h) = A(1 - e^{-\frac{(h/B)^2}{2}})
$$

```matlab
function output = wsq(args);
global pts vario np;
range = args(1);
sill = args(2);
theor = sill * (1 - exp(-(pts/range).^2));
output = sum(((theor - vario)./theor).^2.*np);
```

The above function is kept in a separate file \texttt{wsq.m}

The next part is applied after the empirical variogram is calculated (it is kept in variable \texttt{g}).

```matlab
global pts vario np; % we use them later for the function wsq
pts = g(2:end,3); % bin centers
vario = g(2:end,4); % values of gamma
np = g(2:end,5); % number of points in each variogram bin
[pars,fval] = fminsearch(@wsq,[80, 55])
```

We later plot the empirical variogram along with the fit to see if this particular model is satisfactory.
Exercises:

1. The following were generated from Exponential and Gaussian models, with or without nuggets (f.y.i., plot C is from Sine Wave model). For each of the plots below except C, try to guess which model is used and the approximate values of parameters. [To develop some understanding of the shapes, make your own simulations from different models. Hint: there are two with nuggets.]
2. Do the exercise 3.4 (p. 63) in Kitanidis.
3. Simulate a realization of 1-d Brownian motion with \( n = 1000 \), and obtain its empirical variogram. Would you have guessed, looking at the plot, that it came from a linear variogram model?

4. Repeat the fitting exercise for CaMg data using spherical model. Use a couple of different bin choices for the empirical variogram. Which model seems to fit better, Gaussian or spherical?

5. Plot the empirical variogram for the residuals from High Plains aquifer quadratic fit (data set used in Lab 1 and Lecture 8). Although we have seen possible anisotropy, try and fit an isotropic variogram. Which model would you suggest we use for fitting it?