Module 12 Geostatistics - Lesson 4
Ordinary kriging

June 2018

1 Aim

To introduce ordinary kriging (OK) as a special case of the regression model.

2 Learning outcomes

At the end of the lesson you should be able to:

- explain the difference between the sample mean and spatial mean;
- define and explain the "BLUP" in the context of kriging;
- discuss the the ordinary kriging predictor and identify and explain the two terms in the equation;
- discuss the ordinary kriging variance and identify and explain the three terms in the equation;
- identify the relationship between the sample structure and (1) the weights for the predictor and (2) the kriging variance;
- implement a simple example in R/gstat and evaluate the results.

3 Overview

The day has the following format:

Task	Mandatory / Optional	Time allocation (hrs)
Review of yesterday	Mandatory	1
Lecture	Mandatory	2
Reading	As required	As required
Practical exercise	Mandatory	4

Webster and Oliver [2007] includes a chapter on kriging, although we do not recommend it. Instead we recommend Diggle and Ribeiro Jr. [2007] Chapter 6. Pebesma [2006] is an accessible paper that links well to next week's lesson on regression kriging. Stein and Corsten [1991] is a more detailed paper that links to next week's topics on regression kriging and cokriging. It is an advanced paper and it is not required to read it, although it may be of interest to students who wish to take the topic further.

The relevant parts from Diggle and Ribeiro Jr. [2007] are:

- Sections 6.2 (not 6.2.3 and 6.2.4) and 6.4 are the most useful sections. Please read these sections.
- Section 6.1 is useful, but not essential.
- Section 6.3 discusses the nugget effect and goes beyond what is needed for this class.

4 Assessment

This practical exercise is not formally assessed. However, you are required to complete it. Group 5 should present the findings from today's practical exercise. Group 4 should pose questions.

5 Practical exercise

5.1 Ordinary Kriging (OK) on the Jura dataset

For this part we will build on the work that you did yesterday. There you estimated the sample variogram and fitted a model for nickel for the Jura dataset.

To begin with, load the required libraries.

```
> require(gstat)
> require(sp)
> require(rgdal)
> require(maptools)
```

Load the data. Today we will also use `jura.val` (for validation) and `jura.grid` (which provides a grid for mapping). As before we remove data associated with the Argovian rock type.

```
> rm(list=ls())
> load("jura.rda")
> jura.pred <- jura.pred[jura.pred$Rock!="Argovian",]
> #head(jura.pred)
> dim(jura.pred)

[1] 206  13

> jura.val <- jura.val[jura.val$Rock!="Argovian",]
> #head(jura.val)
> dim(jura.val)

[1] 77 13
```

for validation

Assign the coordinates and convert the data frames to `sp` objects.

```
> jura.pred.df <- jura.pred
> coordinates(jura.pred) <- ~Xloc + Yloc
> jura.val.df <- jura.val
> coordinates(jura.val) <- ~Xloc + Yloc
> jura.grid.df <- jura.grid
> coordinates(jura.grid) <- ~Xloc + Yloc
```

provide a grid for mapping

5.1.1 Variogram modelling

Fit the variogram model. This is demonstrated briefly below, but you should should build on what you learnt yesterday.

```
> ni.ev <- variogram(Ni~1, data=jura.pred)
> ni.mv <- fit.variogram(ni.ev,  model=vgm(70, "Sph", 1, 15), fit.method=7)
> plot(ni.ev, ni.mv)
```

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5.1.2 Ordinary kriging at one unsampled location

We first use OK to predict Nickel concentration at one unsampled location $\mathbf{u}_0$ with coordinates (2.6,3.6) (local coordinate system). We use the `krige` command:

```
> Y0     <- SpatialPoints(data.frame("Xloc"=2.6,"Yloc"=3.6))
> Y0.ok  <- krige(Ni~1, loc=jura.pred, newdata=Y0, model=ni.mv)

[using ordinary kriging]

> Y0.ok

  coordinates var1.pred var1.var
1  (2.6, 3.6)  6.739457 22.59993
```

predicted value at unsampled location (2.6,3.6)

kriging variance=variance(T_hat-T)

We get two outputs: the kriging predictor at location $\mathbf{u}_0$ (`var1.pred`) and the kriging variance at location $\mathbf{u}_0$ (`var1.var`).

5.1.3 Ordinary kriging on a regular grid

We now want to predict nickel concentrations on a regular grid of unsampled locations in order to create a map. We first create a regular grid of points that covers approximately the same area as the measurements, with 50 m spacing:

```
> grid  <- expand.grid(Xloc=seq(0.3, 5.1, by=0.05), Yloc=seq(0.1, 5.9, by=0.05))
> grid  <- SpatialPoints(grid)
> gridded(grid)  <- TRUE
> head(grid)

Object of class SpatialPixels
Grid topology:
     cellcentre.offset cellsize cells.dim
Xloc               0.3     0.05        97
Yloc               0.1     0.05       117
SpatialPoints:
     Xloc Yloc
[1,] 0.30  0.1
[2,] 0.35  0.1
[3,] 0.40  0.1
[4,] 0.45  0.1
[5,] 0.50  0.1
[6,] 0.55  0.1
Coordinate Reference System (CRS) arguments: NA
```

We can plot this grid along with the locations of the measurements:

```
> plot(grid, axes=T)
> plot(jura.pred, col='red', add=T)
```

The constant, unknown spatial mean needs to be estimated

We can now implement ordinary kriging using the `krige` command:

```
> jura.ok  <- krige(Ni~1, loc=jura.pred, newdata=grid, model=ni.mv)
```

```
[using ordinary kriging]
```

We now plot the results (kriging predictions and kriging variance). The measurement locations are overplotted.

```
> X11()
> spplot(jura.ok, "var1.pred", sp.layout=list("sp.points", pch=19, col="green", jura.pred),
+ main="Kriged predictions of Ni (Jura)")
> X11()
> spplot(jura.ok, "var1.var", sp.layout=list("sp.points", pch=19, col="green", jura.pred),
+ main="Kriging variance of Ni (Jura)")
```

Note that the kriging variance increases as we go further from the sample points. Note also that the kriged prediction tends towards the spatial mean as we move further from the sample points.

the degree that prediction is deviated from true value.

5.1.4 Validation

We can use cross-validation to assess the bias and accuracy of our predictions, as follows

```
> jura.cv <- krige.cv(Ni~1, jura.pred, model=ni.mv)
> str(jura.cv)
```

We can calculate the mean error (ME: bias) and root mean square error (RMSE: accuracy)

```
> me <- sum(jura.cv$residual) / length(jura.cv$residual)
> mse <- sum(jura.cv$residual^2) / length(jura.cv$residual)
> rmse <- sqrt(mse)
```

In general the ME should be close to zero (unbiased predictions) and the RMSE should be low (accurate predictions). You can assess the impact of chosing a different variogram model (`ni.mv`) on the prediction ME and RMSE. This may help you to make a choice of variogram model.

An alternative to cross validation is to validate your predictions against a separate datasets. We could split our dataset in two, one part for estimating the variogram and for prediction and the other for validation. THe Jura dataset has already been split, and `jura.val` is provided for validation. We can perform kriging at the locations in `jura.val` and then compare the predicted values to the measured values.

```
> jura.val.ok  <- krige(Ni~1, loc=jura.pred, newdata=jura.val, model=ni.mv)
```

```
[using ordinary kriging]
```

```
> # Calculate the error, rmse and mean error
> jura.err <- jura.val.ok$var1.pred - jura.val$Ni
> me <- sum(jura.err) / length(jura.err)
> mse <- sum(jura.err^2) / length(jura.err)
> rmse <- sqrt(mse)
```

5.2 Part 2: spreadsheet

In this practical we will use a spreadsheet to demonstrate the ordinary kriging theory. The spreadsheet can be downloaded from Blackboard (Day 4).

5.2.1 Description of the spreadsheet

The spreadsheet is composed of 5 parts.

Variogram As an example, we use in the spreadsheet an exponential variogram model. In this part of the spreadsheet you can specify the values of the three variogram parameters: (partial) sill σ^2, nugget τ^2 and range ϕ. The semi-variance $\gamma(\mathbf{h})$ for two points separated by a lag distance $\mathbf{h}$ is:

$$\gamma(\mathbf{h}) = \begin{cases} 0 & \text{if } \mathbf{h} = 0 \\ \tau^2 + \sigma^2 \left(1 - e^{-\frac{h}{\phi}}\right) & \text{if } \mathbf{h} > 0 \end{cases}$$

Points In this part of the spreadsheet, you can specify the set of observations and the set of points to be predicted with kriging. There are 6 sampled locations (top table), denoted points A to F; you can modify their coordinates (X, Y) as well as their observed values. The vector of observed values is denoted $\mathbf{y}$ in this morning lecture. There are 7 unsampled locations (bottom table), denoted points a to g: you can also modify their coordinates (X, Y). The last two columns in the bottom table give you the value of the kriging predictor $\hat{T}$ and the kriging variance $Var\left(\hat{T} - T\right)$ for each unsampled location: have a look at the formulas.

Lag distances To perform ordinary kriging, one first need to compute the lag vector $\mathbf{h}$ for each pair of sampled points A to F (to further get the covariance matrix $\mathbf{C}$), as well as the lag vectors $\mathbf{h}$ between each sampled point (A to F) and each point to be predicted (a to g). These lag distances are simply computed from the point coordinates and are given in two matrices in this part of the spreadsheet.

Kriging computation In this part of the spreadsheet, you will find the core calculations of the kriging system. Top-left matrix is the covariance matrix $\mathbf{C}$, simply derived from the matrix of lag distances $\mathbf{h}$ between sample points A to F and the exponential variogram parameters σ^2, τ^2 and ϕ:

$$C(\mathbf{h}) = C(0) - \gamma(\mathbf{h}) = \begin{cases} \tau^2 + \sigma^2 & \text{if } \mathbf{h} = 0 \\ \sigma^2 e^{-\frac{\mathbf{h}}{\phi}} & \text{if } \mathbf{h} > 0 \end{cases}$$

Top-right matrix gives, for each unsampled location a to g, the covariance $C(\mathbf{h})$ between all observations and the unsampled location (vector $\mathbf{c}_0$ in the lecture). These values are computed from the lag distances $\mathbf{h}$ using the variogram equation. Below the covariance matrix, you will find the value of the spatial mean $\hat{\mu}$, which is given by:

$$\hat{\mu} = \left(\mathbf{1}^T \mathbf{C}^{-1} \mathbf{1}\right)^{-1} \mathbf{1}^T \mathbf{C}^{-1} \mathbf{y}$$

where $\mathbf{y}$ is the vector of observed values and $\mathbf{1}$ is a vector of 1's of length $n = 6$. Finally, the bottom-right matrix from this part of the spreadsheet gives, for each unsampled location a to g to be predicted, the kriging weights λ_i associated to the observed values at sampled points A to F.

Plots of kriging weights This contains seven plots that show, for each unsampled location a to g, the kriging weights λ_i associated to each observed points.

Kriging variances This part gives a table with the predicted valus and kriging variances (variance of the prediction error) for each of the points to be predicted. It also gives a figure showing the kriging variances.

Decomposition of formulae This part gives the decomposition of the kriging predictor (two terms) and kriging variance (three terms). These are also illustrated graphically.

5.2.2 Effect of the variogram range

We will first investigate the effect of the variogram range a on the kriging results. Follow these steps:

1. Select one of the unsampled point within the grid: point a $(1, 1)$, b $(2, 1)$ or c $(1, 2)$
2. Change the variogram range a to 0.2
3. Note the change in predicted value and kriging variance at the selected point
4. Observe the change in kriging weights
5. Repeat this for range values equal to 0.4, 0.6, 1.0, 1.5, 2.5, 5 and 25
6. Make a graph with the range on the x-axis and the predicted value on the y-axis.
7. Make a graph with the range on the x-axis and the kriging variance on the y-axis.

Describe and explain your observations. Then repeat the exercise above for an unsampled point that is not too far outside the observation area, for example point f $(-1, -1)$ or point $(2, 3)$. You should also look at what happens when the point to be predicted is at the same location as a sampled point. Explain your observations.

5.2.3 Effect of the sill and nugget parameters

We will now investigate the effect of both the sill σ^2 and nugget τ^2 parameters on kriging variance. We will keep the total sill $\sigma^2 + \tau^2$ constant. What we will modify is only the ration of spatial variation (sill parameter) to that of the non-spatial variation (the nugget). Investigate the effect of the ratio of spatial variation (sill parameter) to that of the non-spatial variation (the nugget).

1. Take values (5,0) (nugget, partial sill). You should fix the range parameter at 2.
2. Take the same internal point as above (i.e., (1, 2), (2, 1) or (1, 1).
3. Predict the values and determine the kriging variance.
4. Repeat this for the combinations (4, 1), (2.5, 2.5), (1, 4) and (0, 5) for the pair (nugget, partial sill). Note that, in all cases the total sill is 5.
5. Repeat this for the same external point as above (i.e., (-1, -1) or (2, 3)).
6. Make a graph with the nugget on the x-axis and the predicted value on the y-axis.
7. Make a graph with the nugget on the x-axis and the kriging variance on the y-axis.
8. Describe and explain your observations.

5.2.4 Difference between sample mean and spatial mean

Calculate the sample mean (mean of observed values at points A to F). Is there a difference with the spatial mean which is computed in the spreadsheet? Explain your answer.

5.2.5 Decomposition of the kriging predictor and the kriging variance

As shown this morning: decompose the kriging variance into its three constituting elements, and split the equation for the predicted value into its 2 constituting components.

1. Take values along a line from left to right through the area, i.e., prediction points equal to (-3,1), (-2,1), (-1,1),... , (4,1), (5,1).
2. Make a graph in which you display the 1st, 2nd and 3rd component of the kriging variance as a function of the x-coordinate of the prediction point
3. Do the same for the two components of the predicted value.
4. Describe and explain your observations.

6 Tasks and questions

1. Define "BLUP". Give a brief outline of this concept.
2. Complete Part 1. Why does the kriging variance increase as we go further from the sample points? Why does the kriged prediction tend towards the spatial mean as we move further from the sample points? Explain this in terms of the equations for the kriged prediction and kriging variance.
3. You performed two types of validation. First you performed cross-validation and then quantified bias and accuracy using the ME and RMSE. Next you used a separate dataset and quantified bias and accuracy in the same way. Did you obtain similar or different results. Explain this.
4. Look at your result from Lesson 3. Take your preferred and least preferred model and use these to perform kriging. Calculate the ME and RMSE for both validation methods and compare the results. Explain these results.
5. Complete the tasks outlined in Part 2 and answer those questions.

References

P. J. Diggle and P. J. Ribeiro Jr. *Model-based Geostatistics*. Springer, New York, 2007.

E. Pebesma. The role of external variables and gis databases in geostatistical analysis. *Transactions in GIS*, 10:615–632, 2006.

A. Stein and L. C. A. Corsten. Universal kriging and cokriging as a regression procedure. *Biometrics*, 47:575–587, 1991.

R. Webster and M. Oliver. *Geostatistics for Environmental Scientists*. John Wiley and Sons, Chichester, second edition, 2007.