Modeling Spatially Continuous Data

Interactive Spatial Data Analysis
Bailey and Gatrell- Chapter 5

Lecture 14

October 22, 2009

Model Construction

- Construct specific models to explain observed variation in an attribute value over the region R

Models for first order effects

Trend surface analysis

Mean is represented as a polynomial function of a specified order

Polynomial functions of the spatial coordinates of sample sites are fit to observed data values at these sites by ordinary least squares regression

Covariates other than coordinates can be included in the regression

Trend Surface Analysis

- Observation data (z_i) are approximated by a polynomial expansion of the geographic coordinates of the sample points
- Each original observation is considered to be the sum of the polynomial function of the geographic coordinates plus a random error.

$$z_i = f\left(x_i, y_i\right) + e_i$$

$$z_i = b_0 + b_1 x_i + b_2 y_i + e_i$$

Trend Surface Analysis

Conventional multiple regression model in vector notation

$$Z(s) = \underbrace{x^T(s)\beta}_{\text{Mean value or trend}} + e(s) \longleftarrow$$

Zero mean random variable representing fluctuations from the trend

x(s) is a p x 1 vector of p functions of the spatial coordinates

β is a p x 1 vector of coefficients to be estimated

- For a linear trend surface the p functions are: $(1,x,y)^T$
- For a quadratic trend surface these are: $(1, x, y, x^2, xy, y^2)^T$

$$nb_0 + b_1\sum_{i=1}^{n} X_i = \sum_{i=1}^{n} Y_i \qquad b_0\sum_{i=1}^{n} X_i + b_1\sum_{i=1}^{n} X_i^{\,2} = \sum_{i=1}^{n} X_i Y_i$$

Normal equations

$$\mathbf{X}'\mathbf{X} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ X_1 & X_2 & X_3 & X_4 \end{bmatrix} \begin{bmatrix} 1 & X_1 \\ 1 & X_2 \\ 1 & X_3 \\ 1 & X_4 \end{bmatrix} = \begin{bmatrix} n & \sum X_i \\ \sum X_i & \sum X_i^{\,2} \end{bmatrix}$$

$$\mathbf{X}'\mathbf{Y} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ X_1 & X_2 & X_3 & X_4 \end{bmatrix} \begin{bmatrix} Y_1 \\ Y_2 \\ Y_3 \\ Y_4 \end{bmatrix} = \begin{bmatrix} \sum Y_i \\ \sum X_i Y_i \end{bmatrix}$$

Normal equations can be written as

$$\mathbf{X}'\mathbf{X}\mathbf{b} = \mathbf{X}'\mathbf{Y} \qquad \mathbf{b} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$$

Trend Surface Analysis

Assumptions about errors:

e(s) have a constant variance and are independent - covariance is zero

No second order effects in the process Y(s)

Under this assumption the model can be fit by ordinary least squares

Estimate coefficients β and their standard errors

$$\hat{\boldsymbol{\beta}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y} \qquad VAR(\hat{\boldsymbol{\beta}}) = \sigma^2(\mathbf{X}^T\mathbf{X})^{-1}$$

Trend Surface Analysis

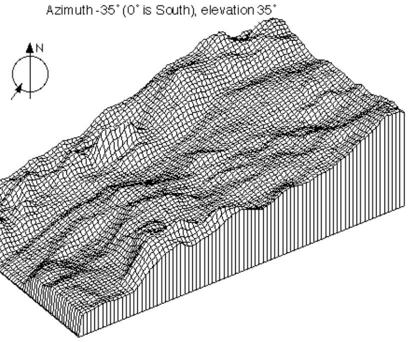
X is a (n x p) matrix with row vectors $x^T(s_i)\ i = 1,\dots.n$

For example for a quadratic trend surface

$$\mathbf{X} = \begin{pmatrix} 1 & x_1 & y_1 & x_1^2 & y_1^2 & x_1y_1 \\ 1 & x_2 & y_2 & x_2^2 & y_2^2 & x_2y_2 \\ 1 & x_n & y_n & x_n^2 & y_n^2 & x_ny_n \end{pmatrix}$$

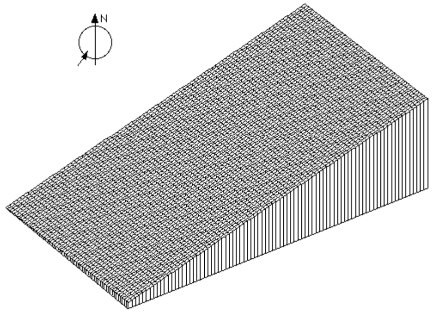
Bouguer gravity, northwest Kansas

Azimuth -35° (0° is South), elevation 35°



http://www.kgs.ukans.edu/Tis/surf3/s3trend2.html

The first-order polynomial of the gravity data set shows the strong east-to-west gradient.

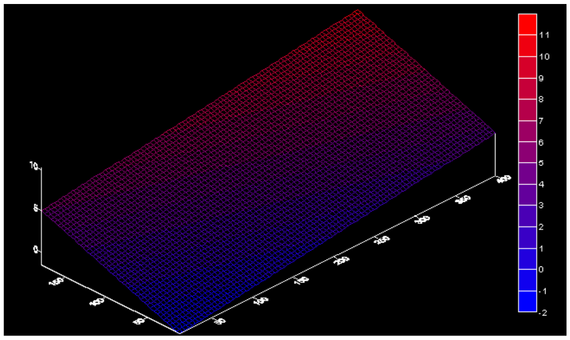


Bouguer gravity, first-order trend, northwest Kansas

Azimuth -35° (0° is South), elevation 35°

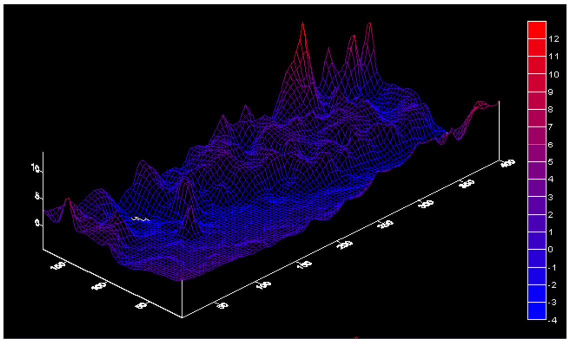
http://www.kgs.ukans.edu/Tis/surf3/s3trend2.html

First Order Trend Surface

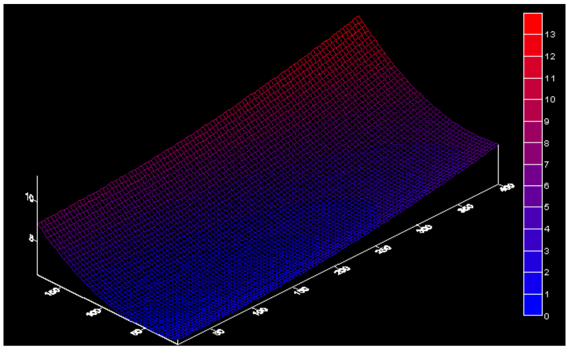


http://filebox.vt.edu/users/smwarner/www/

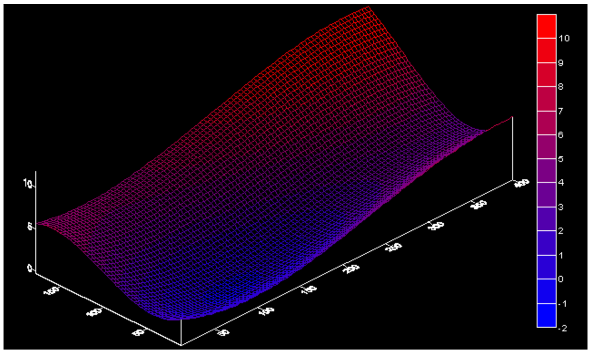
Residuals from First Order Trend Surface



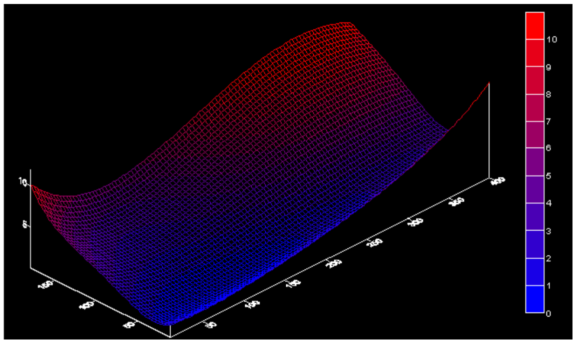
Second Order Trend Surface (1, x, y, x^2, y^2 , xy$)^T$



Third Order Trend Surface $(1, x, y, x^2, y^2, xy, x^3, y^3, x^2y, xy^2)^T$



Fourth Order Trend Surface



Evaluating a Trend Surface

- Test whether a particular surface is different than random.

  i.e. the spatial distribution of the dependent variable is not random or not independent of location.

- Null hypothesis - all coefficients are zero (no trend effect) or all coefficients beyond the k terms of surface order p are statistically equal to zero

  $H_0 = b_1 = b_2 \ldots b_k = 0$

  H_a: $b_1 \neq 0, b_2 \neq 0$, ...and/or $b_k \neq 0$ (at least one coef. is nonzero)

- Rejecting the null hypothesis implies that the regression fit is significant (i.e., it is meaningful and provides a reasonable model for the regional trend of the data set)

Evaluating a Trend Surface

- A trend surface can be evaluated for its statistical significance by dividing the mean square due to the regression by the mean square due to the deviation.
- The result of the quotient is the F test value.
- Find critical F statistic in a table using the degrees of freedom and an alpha value.

General ANOVA for significance of regression of k^{th} degree polynomial trend surface

Source of variation	Sums of squares	Degrees of freedom	Mean Square	F-test
Regression	SS_R	m	$MS_R = SS_R/m$	MS_R / MS_D[1]
Residual	SS_{Rp}	N-m-1	$MS_D = SS_{Rp}/N\text{-}m\text{-}1$	
Total	SS_T	N-1		

where
m is the number of trend coefficients (excluding b_0)
N is the number of data points

[1] Tested against tabled values of F at the chosen significance level

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Evaluating a Trend Surface

- The significance of increasing from one surface to the next higher order surface can also be evaluated with the F test.
- The Mean Square of the regression due to the increase in order is divided by the mean square of the deviation from the higher order surface to calculate the F test value, which again is assigned a F statistic based on the degrees of freedom and alpha value.

Source of variation	**Sums of squares**	**Degrees of freedom**	**Mean Square**	**F-test**
Regression (p+1)	SS_{Rp+1}	m	MS_{Rp+1}	[1]MS_{Rp+1} / MS_{Dp+1}
Deviation (p+1)	SS_{Dp+1}	N-m-1	MS_{Dp+1}	
Regression p	SS_{Rp}	k	MS_{Rp}	[2] MS_{Rp} / MS_{Dp}
Deviation p	SS_{Dp}	N-k-1	MS_{Dp}	
Increase p to p+1	$SS_{Ri} = SS_{Rp+1} - SS_{Rp}$	m-k	MS_{Ri}	[3] MS_{Ri}/MS_{Dp+1}
Total	SS_T	N-1		

k is the number of trend coefficients (excluding b_0) for degree p
m is the number of trend coefficients (excluding b_0) for degree p+1
N is the number of data points

[1] Test of significance of surface order (p+1)
[2] Test of significance of surface order p
[3] Test of significance of increase of fit for (p+1) surface over p-degree surface; test against tabled values of F at the chosen significance level

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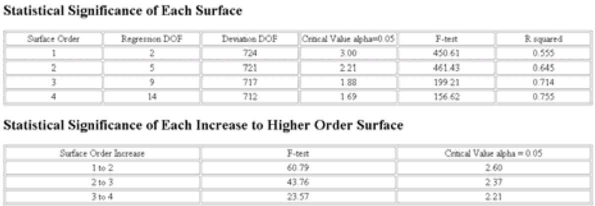


Statistical Significance of Each Surface

Surface Order	Regression DOF	Deviation DOF	Critical Value alpha=0.05	F-test	R squared
1	2	724	3.00	450.61	0.555
2	5	721	2.21	461.43	0.645
3	9	717	1.88	199.21	0.714
4	14	712	1.69	156.62	0.755

Statistical Significance of Each Increase to Higher Order Surface

Surface Order Increase	F-test	Critical Value alpha = 0.05
1 to 2	60.79	2.60
2 to 3	43.76	2.37
3 to 4	23.57	2.21

Trend Surface Analysis

There are a number of disadvantages to trend surface models

- The polynomial surface is extremely simple in form compared to most natural surfaces
- A trend surface generally cannot pass through the data points, rather it has the characteristics of an average.
- The expectation is that the errors are normally distributed, independent, with a mean of zero and a constant variance that depends neither on the parameters $ß_i$ nor the variables X_i

Evaluation of Trend Surface

Examination of residuals to assess the model fit

- The covariogram, variogram or correolgram can be used to examine spatial dependencies in the residuals
- The degree of spatial dependence can be an indicator of how suspect parameter estimates and standard errors may be

Evaluation of Trend Surface

Autocorrelation in the residuals effects significance testing of the trend surface

- The F-test requires an assessment of the degrees of freedom in the data.
- This is defined as the number of independent data values
- Residual autocorrelation tends to reduce the true number of independent data values
- The consequence is an increase in the computed F-value and the probability of committing a Type I error - that is, rejecting a correct null hypothesis and accepting for interpretation a surface that is not really significant

Generalized Least Squares

A regression technique that is used when the error terms from an ordinary least squares regression display non-random patterns such as autocorrelation or heteroskedasticity.

The model is then

$$Y(s) = x^T(s)\beta + U(s)$$

Where U(s) are zero mean errors but they are not independent and have covariance function C()

Estimates for the coefficients β and standard errors become

$$\hat{\beta} = (X^T C^{-1} X)^{-1} X^T C^{-1} y$$

$$VAR(\hat{\beta}) = (X^T C^{-1} X)^{-1}$$

Generalized Least Squares

C is an (n x n) matrix of covariances between the residuals $U(s_i)$ and $U(s_j)$ for each possible pair of the *n* sample locations. Diagonal elements of the matrix are the variances of the residuals.

- Generalized least squares provides a model for both first and second order effects $Y(s) = x^T(s)\beta + U(s)$
- Problem is the covariance matrix is unknown.
- Need a model of covariance structure that can be estimated from the data

Models for Variograms

The semivariance is a measure of the degree of spatial dependence between samples.

Since only the semivariance at certain points is known, a variogram model needs to be fitted through the variogram values to get the semivariance value at all points (distances)

Models for Variograms

Seek smooth continuous model of covariance that can be fit to the sample variogram

- This model can then be used to estimate the covariance matrix C for generalized least squares model
- Must assume some form of stationarity to develop such models
- If there is evidence of trend, the trend should be removed using regression methods and apply the model to the residuals

Iterative Approach

1. Remove trend by ordinary least squares
2. Use residuals to model covariance structure
3. Re-estimate trend using generalized least squares with estimated covariance structure

Models for Variograms

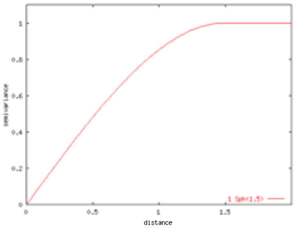
Constraints for valid variogram models

Symmetry $C(s_i, s_j) = C(s_j, s_i)$

Positive Definiteness $\sum_{i=1}^{n}\sum_{j=1}^{n}\alpha_i\alpha_j C\left(s_{i,}s_j\right)\geq 0$

Families of valid variogram models

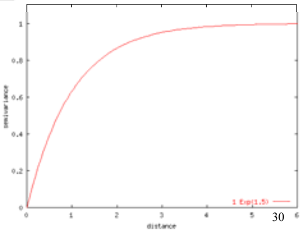
- spherical
- exponential
- Gaussian
- linear



Spherical

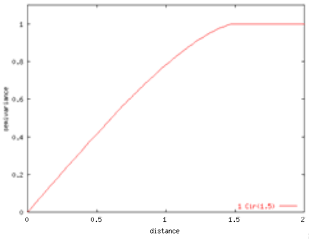
σ^2 is the sill
r is the range

$$\gamma(h)=\begin{cases}\sigma^2(\frac{3h}{2r}-\frac{h^3}{2r^3}) & for\ h\leq r\\ \sigma^2 & otherwise\end{cases}$$



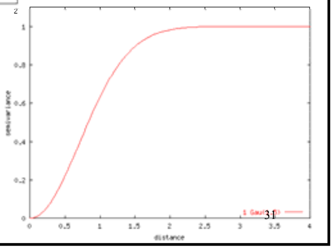
$$\gamma(h)=\sigma^2(1-e^{-3h/r})$$

Exponential



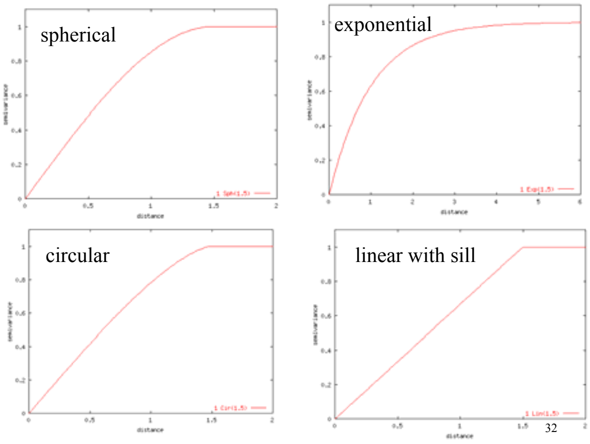
Circular

$$\gamma(h)=\frac{2h}{r\pi}\sqrt{1-\left(\frac{h}{r}\right)^2}+\frac{2}{\pi}\arcsin\frac{h}{r}$$



$$\gamma(h)=\sigma^2\left(1-e^{-3h^2/r^2}\right)$$

Gaussian



Models for Variograms

The nugget variance is that part of the variance of the regionalized variable that has no spatial component (variation due to measurement errors and short-range spatial variation at distances within the smallest inter-sample spacing).

Partial sill is difference between sill and nugget

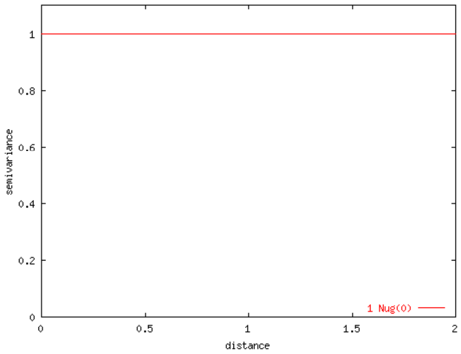
Relative nugget effect

Ratio of nugget effect to the sill

A variogram model can consist of pure nuggett effect

Indicates complete lack of spatial dependence

Variogram of pure nugget effect



Models for Variograms

r is the range

σ^2 is the sill

a is nugget

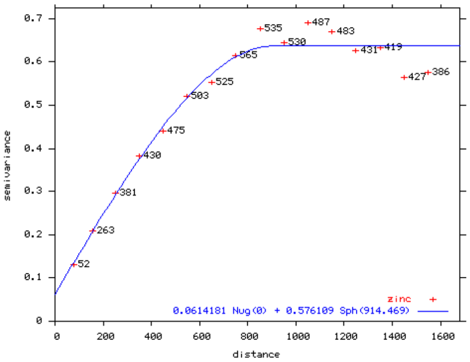
Addition of nugget effect to models

Spherical model

$$\gamma(h) = \begin{cases} a + (\sigma^2 - a)\left(\frac{3h}{2r} - \frac{h^3}{2r^3}\right) & for\ 0 < h \le r \\ 0 & h = 0 \\ \sigma^2 & otherwise \end{cases}$$

Exponential model

$$\gamma(h) = \begin{cases} a + (\sigma^2 - a)(1 - e^{-3h/r}) & h > 0 \\ 0 & h = o \end{cases}$$



Fitted spherical variogram with nugget effect

Models for Variograms

Models for anisotropic structures

h in previous models replaced by distance, direction vector ***h***

Geometric anisotropy

Range changes with direction but sill remains constant

Zonal anisotropy

Sill changes with direction but range remains constant

Models for Variograms

The objective of variogram modeling is to capture the basic structure of spatial dependence

Do not want to overfit the model to the sample variogram as there will be inaccuracies in the sample variogram