空間分析方法與應用 (Geog 5069) | 台大地理系 Spatial Analysis: Methods and Applications

# 地理統計概述

# **Geostatistics: A Brief Introduction**



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授課大綱:地理統計概述

Spatial Interpolation/Prediction

- Stochastic (geostatistics)
  - Semivariogram and Kriging Method
- Deterministic and Non-parametric
  - Inverse Distance Weighting (IDW)



# Geostatistics: Principles of Spatial Interpolation



Z(x): a regionalized random variable that is associated with a true measurement, z(x), that characterizes the quantity of a variable at point x.

# **Spatial Covariance vs. Variogram**

- Spatial Covariance: how that variable is distributed across space, focusing on the degree of similarity among pairs of data points.
- We can define the values of the random variable Z at two locations, Z(x) and Z(x + h), where h represents the distance (spatial lag) between a pair of sampling sites.

$$C(h) = E[Z(x+h).Z(x)] - \mu^2$$
  
where  $\mu$  is the stationary mea

# **Spatial Covariance Function**

```
spatial structure of the data
assumption of stationary covariance
C(h) = \mathbb{E}[Z(x+h).Z(x)] - \mu^2
 C(h)
                However, it cannot be estimated directly
```

۰h

# Variogram

A variogram might be thought of as "dissimilarity between point values as a function of distance", such that the dissimilarity is greater for points that are farther apart



# **Variogram: Mathematical definition**

$$2\gamma(h) = E\left\{ [Z(x+h) - Z(x)]^2 \right\}$$

$$2\gamma(h) = average\left[ (Z(i) - Z(j))^2 \right]$$

$$2\hat{\gamma}(h) = \frac{1}{N(h)} \sum_{N(h)} (Z(s_i) - Z(s_j))^2$$

N(h): the number of paired comparisons at lag h.



$$\gamma(h) = \frac{1}{2n(h)} \sum_{i=1}^{n(h)} \left[ z(x_i + h) - Z(x_i)^2 \right]$$

where *n* is the number of sample points,  $Z(x_i)$  is the measured sample value at location  $x_i$ ,  $Z(x_{i+h})$  is the sample value at location  $x_{i+h}$ , regionalized variable Z(x), and n(h) is the number of pairs of observations a distance *h* apart.



# Concept of Semivariogram



## **Fitting a Variogram Model**

- Now, we're going to fit a variogram model (i.e., curve) to the empirical variogram
- That is, based on the shape of the empirical variogram, different variogram curves might be fit
- The curve fitting generally employs the method of least squares T the same method that's used in regression analysis





### **The Variogram Parameters**

- The variogram models are a function of three parameters, known as the range, the sill, and the nugget.
- Semivariance value where it flattens out is called a "sill."
- The distance range for which there is a slope is called the "neighborhood"; this is where there is positive spatial structure
- The intercept is called the "nugget" and represents random noise that is spatially independent

$$\tilde{\gamma}(h) = \frac{1}{2N(h)} \sum_{u=1}^{N} (z(u) - z(u+h))^2$$





$$\gamma(h) = c_0 + c_1 \left[ \frac{3h}{2a} - \frac{1}{2} \left( \frac{h}{a} \right)^3 \right], \text{ for } 0 < h < a,$$

 $\gamma(h)=c_0+c_1, \quad \text{for } h\geq a,$ 

### exponential model

power function



# spherical model

- the most widely used.
- Monotonically non-decreasing: as h increases, the value of γ(h) does not decrease - i.e., it goes up (until h≤r) or stays the same (h>r)



.

nugget (sill-nugget)  

$$\gamma(h) = c_0 + c_1 \left[ \frac{3h}{2a} - \frac{1}{2} \left( \frac{h}{a} \right)^3 \right], \quad \text{for } 0 < h < a$$

$$\gamma(h) = c_0 + c_1, \quad \text{for } h \ge a,$$

# $\gamma(h) = c \left[ 1 - \exp rac{-3h}{a} ight]$

# exponential model

- similar to the spherical model, but assumes that the correlation never reaches exactly zero, regardless of how great the distances between points are
- In other words, the variogram approaches the value of the sill asymptotically
- Because the sill is never actually reached, the range is generally considered to be the smallest distance after which the covariance is 5% or less of the maximum covariance
- The model is monotonically increasing
  - I.e., as h goes up, so does  $\gamma(h)$

#### **Model Variogram Types**

Value	Model variogram type (from VarModel)	Equation
1	Spherical	$\gamma(h)=c\left[1.5rac{h}{a}-0.5ig(rac{h}{a}ig)^3 ight]$
2	Exponential	$\gamma(h) = c \left[ 1 - \exp rac{-3h}{a}  ight]$
3	Gaussian	$\gamma(h) = c \left[ 1 - \exp\left(rac{-3h}{a} ight)^2  ight]$





# The Wave (Hole-Effect) Model

the waves exhibit a periodic pattern. A non-standard form of spatial autocorrelation applies. Peaks are similar in values to other peaks, and troughs are similar in values to other troughs. However, note the *dampening* in the covariogram and variogram below: That is, *peaks* that are closer together have values that are more correlated than peaks that are father apart (and same holds for troughs).





# **Steps of Variogram Modeling**



(a) sampling locations (n=155) and measured variable

(b) variogram cloud showing semivariances for all pairs

# Steps of Variogram Modeling (cont'd)



(c) semivariances aggregated to lags of about 100 m

(d) the final variogram model fitting

# Lab: Variogram (Exploring data)

### ■ 安裝R套件 gstat



#### Spatial and Spatio-Temporal Geostatistical Modelling, Prediction and Simulation

Variogram modelling; simple, ordinary and universal point or block (co)kriging; spatio-temporal kriging; sequential Gaussian or indicator (co)simulation; variogram and variogram map plotting utility functions.

# Data: 台灣環保署空氣品質測站資料 (shape file)

#### 73 obs. x 16 variables

	SiteNamê	SiteEngNam	AreaName 🌣	County	Township	SiteAddres	÷	TWD97Lon	TWD97Lat	SiteType	Name <sup>‡</sup>	PSI 🔅	PM <sup>‡</sup>	<b>O3</b> <sup>‡</sup>	<b>SO2</b> $^{\diamond}$	<b>CO</b> $^{\diamond}$	NO2 ¢
1	二林	Erlin	中部空品區	彰化縣	二林鎮	彰化縣二林鎮萬合里江山巷1號		120.4097	23.92517	一般測站	二林	62	75	40	5.8	0.47	12.0
2	三重	Sanchong	北部空品區	新北市	三重區	新北市三重區三和路重陽路交口		121.4938	25.07261	交通測站	三重	68	102	0	3.0	1.37	36.0
3	三義	Sanyi	竹苗空品區	苗栗縣	三義鄉	苗栗縣三義鄉西湖村上湖61-1號		120.7588	24.38294	一般測站	三義	45	56	32	1.9	0.36	6.3
4	土城	Tucheng	北部空品區	新北市	土城區	新北市土城區學府路一段241號		121.4519	24.98253	一般測站	土城	62	84	30	1.9	0.51	16.0
5	士林	Shilin	北部空品區	臺北市	北投區	臺北市北投區文林北路155號		121.5154	25.10542	一般測站	士林	50	61	32	1.8	0.41	11.0
6	大同	Datong	北部空品區	臺北市	大同區	臺北市大同區重慶北路三段2號		121.5133	25.06320	交通測站	大同	61	78	0	2.3	0.84	20.0
7	大里	Dali	中部空品區	臺中市	大里區	臺中市大里區大新街36號		120.6777	24.09961	一般測站	大里	42	50	37	2.4	0.62	19.0
8	大園	Dayuan	北部空品區	桃園市	大園區	桃園市大園區中正東路160號		121.2018	25.06034	一般測站	大園	62	85	35	3.3	0.37	12.0
9	大寮	Daliao	高屏空品區	高雄市	大寮區	高雄市大寮區潮寮路61號		120.4251	22.56575	一般測站	大寮	72	109	51	8.2	0.91	38.0
10	小港	Xiaogang	高屏空品區	高雄市	小港區	高雄市小港區平和南路185號		120.3377	22.56583	一般測站	小港	86	132	34	7.1	0.72	31.0
11	中山	Zhongshan	北部空品區	臺北市	中山區	臺北市中山區林森北路511號		121.5265	25.06236	一般測站	中山	52	81	14	2.4	1.06	33.0
12	中壢	Zhongli	北部空品區	桃園市	中壢區	桃園市中壢區延平路622號		121.2217	24.95328	交通測站	中壢	67	83	26	2.4	0.91	23.0
13	仁武	Renwu	高屏空品區	高雄市	仁武區	高雄市仁武區八卦里永仁街555號		120.3326	22.68906	一般測站	仁武	91	144	32	2.7	0.70	26.0
14	斗六	Douliu	雲嘉南空品區	雲林縣	斗六市	雲林縣斗六市民生路224號		120.5450	23.71185	一般測站	斗六	59	71	41	2.5	0.49	14.0
15	冬山	Dongshan	宜蘭空品區	宜蘭縣	冬山鄉	宜蘭縣冬山鄉南興村照安路26號		121.7929	24.63220	一般測站	冬山	50	49	29	2.1	0.33	12.0
16	古亭	Guting	北部空品區	臺北市	大安區	臺北市大安區羅斯福路三段153號		121.5296	25.02061	一般測站	古亭	45	87	21	0.0	0.67	24.0
17	左營	Zuoying	高屏空品區	高雄市	左營區	高雄市左營區翠華路687號		120.2929	22.67486	一般測站	左營	81	117	40	2.5	0.59	17.0
18	平鎮	Pinazhen	北部李品區	桃園市	平鎮區	桃園市平鎮區文化街189號		121.2040	24.95279	一般測站	平鎮	60	71	31	1.6	0.44	12.0



# **Exploring distance vs. variance** $2\gamma(h) = average[(Z(i) - Z(j))^2]$ Dist.(h) vs. $[z(x+h)-z(x)]^2$

# variogram cloud



**Exploring distance vs. variance (R code)**  $2\gamma(h) = average[(Z(i) - Z(j))^2]$  Dist.(h) vs.  $[z(x+h)-z(x)]^2$ 

```
x= coordinates(EPA_STN)[,1]
y= coordinates(EPA_STN)[,2]
```

```
STNDF = cbind(x,y)
dis_STN= dist(STNDF)
```

```
pm= EPA_STN@data[,12]
```

```
PMDF= cbind(pm,pm)
dis_PM = dist(PMDF)
```

```
plot(dis_PM~sqrt(dis_STN))
abline(lm(dis_PM~sqrt(dis_STN)), lwd=3, col='red')
```

# Using variogram() function in R

variogram {gstat}

R Documentation

#### Calculate Sample or Residual Variogram or Variogram Cloud

Description

Calculates the sample variogram from data, or in case of a linear model is given, for the residuals, with options for directional, robust, and pooled variogram, and for irregular distance intervals.

In case spatio-temporal data is provided, the function <u>variograms</u> is called with a different set of parameters.

library(gstat)
pm.vgm = variogram(PM~1, EPA\_STN,cutoff=80000, width=1000)

# Using variogram() function in R

library(gstat)
pm.vgm = variogram(PM~1, EPA\_STN,cutoff=80000, width=1000)
plot(pm.vgm)



# **Fitting a Variogram Model**

fit.variogram {gstat}

### Fit a Variogram Model to a Sample Variogram



Description

Fit ranges and/or sills from a simple or nested variogram model to a sample variogram

Usage

Sill, func. range, nugget

pm.fit = fit.variogram(pm.vgm, model = vgm(1000, "Exp",2000,1)

vgm {gstat}

### Generate, or Add to Variogram Model



Description

Generates a variogram model, or adds to an existing model. print.variogramModel prints the essence of a variogram model.

Usage

```
vgm(psill = NA, model, range = NA, nugget, add.to, anis, kappa = 0.5, ..., covtabl
Err = 0)
## S3 method for class 'variogramModel'
print(x, ...)
as.vgm.variomodel(m)
```

Sill, func. range, nugget

pm.fit = fit.variogram(pm.vgm, model = vgm(1000, "Exp",2000,1)

# library(gstat) pm.vgm = variogram(PM~1, EPA\_STN,cutoff=80000, width=2000) pm.fit = fit.variogram(pm.vgm, model = vgm(1000, "Exp",20000,1) ) plot(pm.vgm,pm.fit)



# Geostatistical Approach to Spatial Interpolation: using semivariogram





# **Basics of Geostatistics: Understanding underlying spatial structures**



- there seems to be a spatial pattern of how the values change;
- values that are closer together are more similar;
  - Iocally, the values can differ without

any systematic rule (randomly)

### **Universal Model of Variation**

# $Z(\mathbf{s}) = Z^*(\mathbf{s}) + \varepsilon'(\mathbf{s}) + \varepsilon''$

### Z\*(s) is the deterministic component

- ε'(s) is the spatially correlated random component
- **ε**" is the pure noise, e.g. the measurement error.

# **Ordinary Kriging**

 $Z(\mathbf{s}) = Z^*(\mathbf{s}) + \varepsilon'(\mathbf{s}) + \varepsilon''$ 

### Assumptions

- □ *Z*(*s*) should be normally distributed
- □ The global structure Z\*(s) is constant and unknown
- Covariance between values of ε'(s) depends only on distance between the points



# **Principle of Spatial Prediction**



$$\hat{z}_{\text{DK}}(\mathbf{s}_0) = \sum_{i=1}^n w_i(\mathbf{s}_0) \cdot z(\mathbf{s}_i) = \lambda_0^{\text{T}} \cdot \mathbf{z}$$

where  $\lambda_0$  is the vector of kriging weights  $(w_i)$ , **z** is the vector of *n* observations at primary locations.

# 不偏估計 unbiased

The weighted linear estimator for location  $s_0$  is:

$$\hat{Z}_0 = \sum_{i=1}^n w_i Z_i \tag{(*)}$$

The estimation error at location  $s_0$  is the difference between the predictor and the random variable modeling the true value at that location:

$$R_0 = \hat{Z}_0 - Z_0 = \sum w_i Z_i - Z_0$$

The bias is:

$$E(R_0) = E(\sum w_i Z_i - Z_0) = \sum E(w_i Z_i) - E(Z_0)$$
  
=  $\sum w_i E(Z_i) - E(Z_0) = \sum w_i \mu - \mu = \mu(\sum w_i - 1)$ 

So, as long as  $\sum w_i = 1$ , the weighted linear estimator (\*) is unbiased.

### However, how to estimate the weight?

# Minimizing the mean squared error (MSE)

Kriging is such a method that determines the weights so that the mean squared error (MSE) is minimized:

$$MSE = E\left((\hat{Z}_0 - Z_0)^2\right)$$

subject to the unbiasedness constraint  $\sum w_i = 1$ .

The final ordinary kriging system is:

$$C \qquad w = D$$

$$\begin{bmatrix} C_{11} & \dots & C_{1n} & 1 \\ \dots & \dots & \dots & \dots \\ C_{n1} & \dots & C_{nn} & 1 \\ 1 & \dots & 1 & 0 \end{bmatrix} \bullet \begin{bmatrix} w_1 \\ \dots \\ w_n \\ \lambda \end{bmatrix} = \begin{bmatrix} C_{10} \\ \dots \\ C_{n0} \\ 1 \end{bmatrix} \Longrightarrow w = C^{-1}D$$

$$(n+1)\times(n+1) \qquad (n+1)\times1 \qquad (n+1)\times1$$

如何求解極端值?

Minimizing 
$$f(x_1, x_2)$$

Subject to 
$$g(x_1, x_2) = 0$$
 (受限於)

**Lagrangian function (L)**  $L(x_1, x_2, \lambda) = f(x_1, x_2) + \lambda g(x_1, x_2)$ 

$$\frac{\partial L}{\partial x_1} = 0, \ \frac{\partial L}{\partial x_2} = 0, \ \frac{\partial L}{\partial \lambda} = 0$$

Lagrange multiplier

# **Kriging Method**

Assume we have a model:

$$Z(s) = \mu + \varepsilon(s),$$



The weighted linear estimator for location  $s_0$  is:

$$\hat{Z}_0 = \sum_{i=1}^n w_i Z_i$$

$$\begin{split} \Gamma & w &= D \\ \begin{bmatrix} 0 & \gamma_{12} & \dots & \gamma_{1n} & 1 \\ \gamma_{21} & 0 & \dots & \gamma_{2n} & 1 \\ \dots & \dots & \dots & \dots & \dots \\ \gamma_{n1} & \gamma_{n2} & \dots & 0 & 1 \\ 1 & 1 & \dots & 1 & 0 \end{bmatrix} \bullet \begin{bmatrix} w_1 \\ w_2 \\ \dots \\ w_n \\ -\lambda \end{bmatrix} = \begin{bmatrix} \gamma_{10} \\ \gamma_{20} \\ \dots \\ \gamma_{n0} \\ 1 \end{bmatrix} \longrightarrow W = \Gamma^{-1}D \\ (n+1)\times(n+1) & (n+1)\times1 \end{split}$$



**kriging Variance** 



kriging variance in terms of variogram

$$\sigma_{OK}^2 = \sum w_i \gamma_{i0} - \lambda = w'D,$$

# **Ordinary Kriging Estimate and Standard Deviation**



### Ordinary Kriging 計算實例



# 計算資例 Exponential semivariogram model with parameters $c_0 = 0, c_1 = 10, \alpha = 3.33$ .



$$\gamma(h) = 10(1 - e^{-\frac{h}{3.33}}).$$

計算實例 Distance Matrix





# 計算實例 Kriging Weights

	$\begin{pmatrix} 0 \end{pmatrix}$	4.893	9.564	9.800	9.510	9.740	9.952	1)	-1	( 7.384 )
	4.893	0	9.637	9.798	9.093	9.510	<mark>9.938</mark>	1		6.614
	9.564	9.637	0	7.095	9.800	9.889	9.637	1		9.109
$W = \Gamma^{-1} \alpha =$	9.800	9.798	7.095	0	9.755	9.847	8.775	1		9.420
$\mathbf{w} = 1  \gamma =$	9.510	9.093	9.800	9.755	0	4.893	9.775	1		8.664
	9.740	9.510	9.889	9.847	4.893	0	9.806	1		9.316
	9.952	9.938	9.637	8.775	9.775	9.806	0	1		9.823
	\ 1	1	1	1	1	1	1	0 )		$\begin{pmatrix} 1 \end{pmatrix}$

The answer is:



# 計算實例 Kriging Estimate and Variance

The predicted value at location  $s_0$  is equal to:

$$\hat{z}(s_0) = \sum_{i=1}^n w_i z(s_i) = 0.174(477) + \dots + 0.086(783) = 592.59.$$

And the variance:

$$\sigma_e^2 = \sum_{i=1}^n w_i \gamma(s_i - s_0) + \lambda = 0.174(7.384) + \dots + 0.086(9.823) + 0.906 = 8.96.$$

### 95% confidence Interval

 $592.59 \pm 1.96\sqrt{8.96}$ 

#### Or

 $577.09 \le Z(s_0) \le 588.83$ 

# **R Lab: Ordinary Kriging**

krige {gstat}

R Documentation

# Simple, Ordinary or Universal, global or local, Point or Block Kriging, or simulation.

Description

Function for simple, ordinary or universal kriging (sometimes called external drift kriging), kriging in a local neighbourhood, point kriging or kriging of block mean values (rectangular or irregular blocks), and conditional (Gaussian or indicator) simulation equivalents for all kriging varieties, and function for inverse distance weighted interpolation. For multivariable prediction, see <u>gstat</u> and <u>predict</u>

pm.kriged = krige(PM~1, EPA\_STN, grid, model = pm.fit)

# **R Lab: Ordinary Kriging**

- 台灣大學的位置台北市羅斯福路四段1號
- X = 304023
- Y = 2767886

ntu\_pts <-SpatialPoints(cbind(304023,2767886), proj4string = CRS(proj4string(EPA\_STN)))
krige(PM~1, EPA\_STN, ntu\_pts, model = pm.fit)</pre>

# **R Lab: Ordinary Kriging**

建立涵蓋台灣範圍的估計點。 makegrid()

```
# generating grid
proj4string(EPA_STN)
grid <- makegrid(EPA_STN, cellsize = 5000)
grid <- SpatialPoints(grid, proj4string = CRS(proj4string(EPA_STN)))</pre>
```

plot(EPA\_STN)
plot(grid, pch = ".", add = T)



pm.kriged = krige(PM~1, EPA\_STN, grid, model = pm.fit)

spplot(pm.kriged["var1.pred"])
spplot(pm.kriged["var1.var"])



# **Conditional Simulation**

- Spatial mean estimated by kriging.
- Uncertain/stochastic aspect simulated.
- Offers a realistic representation of the variable.
- Gaussian simulations simulated portion follows a normal distribution.





### **Workflow of Geostatistical Estimation**



Directional variogram (e.g. terrain effect)



Space-time variogram



Network structure (e.g. river, road,...)





Regression- Kriging (universal Kriging)

$$\hat{z}(\mathbf{s}_0) = \hat{m}(\mathbf{s}_0) + \hat{e}(\mathbf{s}_0) = \sum_{k=0}^p \hat{eta}_k \cdot q_k(\mathbf{s}_0) + \sum_{i=1}^n \lambda_i \cdot e(\mathbf{s}_i)$$



### Binary outcome variable: Indicator Kriging



### **Deterministic: Inverse Distance Weighting**



Inverse distance weighting (IDW) is a deterministic, nonlinear interpolation technique that uses a weighted average of the attribute (i.e., phenomenon) values from nearby sample points to estimate the magnitude of that attribute at non-sampled locations.



## **R code: Inverse Distance Weighting**

pm.idw = idw(PM~1, EPA\_STN, grid, idp=1)
spplot(pm.idw)











[5.048,36.42] (36.42,67.78] (67.78,99.15] (99.15,130.5] (130.5,161.9]