ÉCOLE POLYTECHNIQUE FÉDÉRALE DE LAUSANNE

Presentation for GSP/NCAR, February 2002

Nonstationarity in Geostatistical Modeling

Reinhard Furrer, IMA, SB, EPF-Lausanne

Outline of the Presentation

- Motivation
- Nonstationarity in the mean
  - Exploratory examination
  - (Non)parametric trend estimation
  - Local trend estimation
  - Simulations and application to SIC97 data
- Nonstationary spatio-temporal processes
  - Construction of nonstationary covariograms
  - Simulations and application to Ozone data
- Conclusion and outlook

Motivation

The spatial process $\{Y(\mathbf{x}) : \mathbf{x} \in \mathcal{D} \subset \mathbb{R}^d, d \geq 1\}$

- is intrinsically stationary if

$$\mathrm{E}\big(Y(\mathbf{x}_i)\big) \equiv \mu$$
$$2\gamma\big(\mathbf{x}_i - \mathbf{x}_j\big) = \mathrm{Var}\big(Y(\mathbf{x}_i) - Y(\mathbf{x}_j)\big)$$

- is second-order stationary if

$$\mathrm{E}\big(Y(\mathbf{x}_i)\big) \equiv \mu$$
$$c\big(\mathbf{x}_i - \mathbf{x}_j\big) = \mathrm{Cov}\big(Y(\mathbf{x}_i), Y(\mathbf{x}_j)\big)$$

There exists many different types of nonstationarity:

- nonstationarity in the mean
- nonstationarity in the second moment structure

Nonstationarity in the Mean

The decomposition based on the scale of variation is

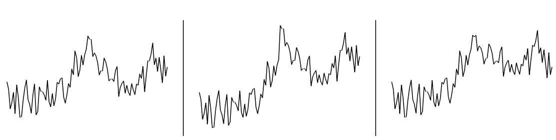
$$Z(\mathbf{x}) = \mu(\mathbf{x}) + Y(\mathbf{x}) + \varepsilon(\mathbf{x}) \qquad \mathbf{x} \in \mathcal{D}$$

with

$\mu(\cdot) = \mathrm{E}\big[Z(\cdot)\big]$ is the deterministic mean structure
$\rightsquigarrow$ large-scale variation
$Y(\cdot)$ is a zero-mean, intrinsically stationary L_2-process
$\rightsquigarrow$ smooth small-scale variation
$\varepsilon(\cdot)$ is a zero-mean white-noise process
$\rightsquigarrow$ measurement error

How to estimate $\mu(\cdot)$?

How to estimate $\mu(\cdot)$?



- Exploratory examination of the process (CUSUM)
- Exploratory examination of the empirical variogram
- Parametric trend estimation
- Nonparametric trend estimation
- Local trend estimation

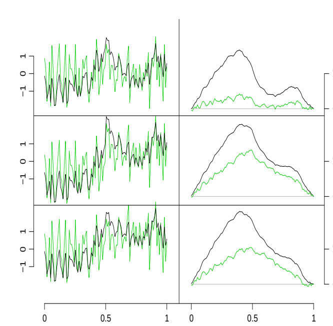
Cumulative Sums (CUSUM)

CUSUM is the series

$$S_K = \sum_{k=1}^{K} Z(x_k) - \bar{Z}, \qquad K = 1, \ldots, n$$

Trend affects the CUSUM.

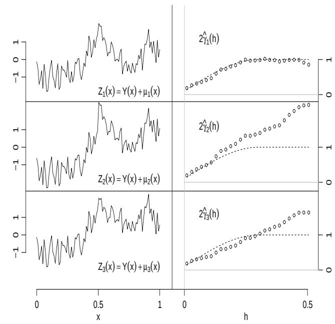
We cannot distinguish between large-scale variation and small-scale variation.



Visual Examination of the Variogram

Trend affects the empirical variogram.

We cannot distinguish between large-scale variation and small-scale variation.



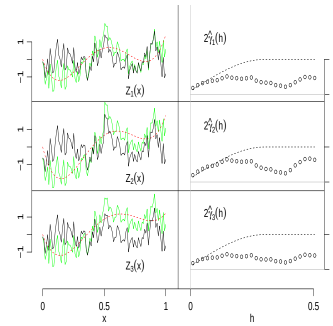
Parametric Trend Estimation

Trend is supposed of the form

$$\mu(\cdot) = \sum_{k=1}^{K} \beta_k g_k(\cdot)$$

How to determine K and the functions $\{g_k(\cdot)\}$?

Significance depends on range and number of locations.



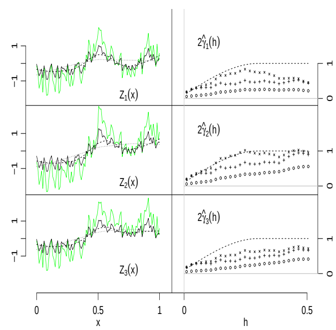
Nonparametric Trend Estimation

Trend is estimated with local regression techniques.

How to determine smoothing or bandwidth parameter?

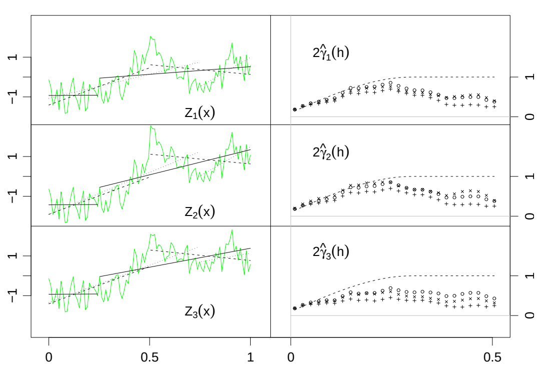
Often too much small-scale variation is extracted.

Empirical variogram depends on smoothing parameter.



Local Trend Estimation

- Localization technique
- Domain is divided (heuristically) into several sub-domains
- Local trends are approximated by linear functions
- Residuals can be pooled for further analysis $\rightsquigarrow$ borrowing strength



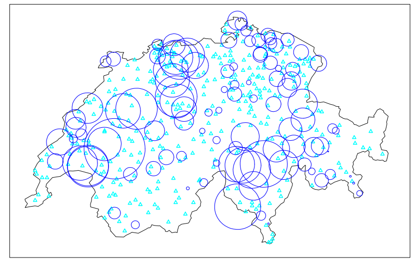
Advantages of the Method

- Subdomains can be heuristically be determined
- In homogeneous setting LTE does no harm
- Empirical variograms are not sensible to the choice of the subdomains
- Easy to implement and not computing intensive
- Can be applied to other characteristics

Weak Points of the Method

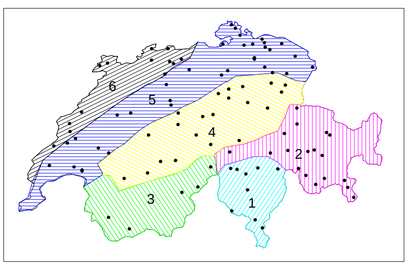
- Fitted surface is not continuous
- Sparse or aligned data may lead to artifacts
- Subdomains can only be heuristically determined

Application: SIC97 Data



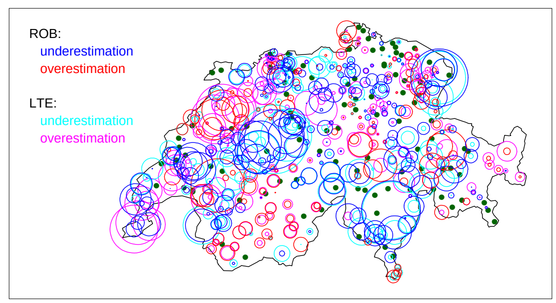
SIC97 data (Spatial Interpolation Contest 1997). Comparison of interpolation methods of 22 participants. Dubois (2000) distributed 100 daily rainfall data to predict at the 367 remaining locations.

Application: SIC97 Data



SIC97 data (Spatial Interpolation Contest 1997). Comparison of interpolation methods of 22 participants. Dubois (2000) distributed 100 daily rainfall data to predict at the 367 remaining locations.

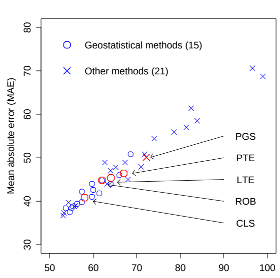
Results



LTE: local trend estimation
ROB: Genton and Furrer (1998a)

Results

Method	LTE	PTE	ROB	CLS	PGS
Practical range	72.9	53.9	39.7	60	—
Scaled sill	0.692	0.853	0.974	1	—
Scaled nugget effect	0.308	0.147	0.026	0	—
Nugget effect/sill	0.446	0.173	0.027	1	—
RMSE	64.08	67.02	62.10	58.08	72.22
MAE	45.38	46.39	44.79	40.89	50.14
MAD	44.80	48.47	48.74	42.73	53.37



LTE: local trend estimation
PTE: polynomial trend estimation
ROB: Genton and Furrer (1998b)
CLS: classical least squares
PGS: Genton and Furrer (1998a)

Nonstationary Spatio-Temporal Processes

The spatio-temporal process

$$\{Y(\mathbf{x},t) : \mathbf{x} \in \mathcal{D} \subset \mathbb{R}^d, t \in \mathcal{T}\}$$

is second-order stationary in space and time if

$$\mathsf{E}\big(Y(\mathbf{x}_i,t_r)\big) \equiv \mu$$
$$c\big(\mathbf{x}_i - \mathbf{x}_j, t_r - t_s\big) = \mathsf{Cov}\big(Y(\mathbf{x}_i,t_r), Y(\mathbf{x}_j,t_s)\big)$$

According to Bochner (1933), Cressie and Huang (1999), a continuous, bounded, symmetric and integrable function $c(\mathbf{h},u)$ is a space-time covariance function if and only if

$$c^{\mathcal{F}}_{\omega}(u) = \int \exp(-\imath \mathbf{h}^{\mathsf{T}}\boldsymbol{\omega})c(\mathbf{h},u)\,d\mathbf{h}$$

is a covariance function for almost all $\boldsymbol{\omega} \in \mathbb{R}^d$.

Nonstationary Covariograms

We write the covariogram of a process which is nonstationary in time as

$$c(\mathbf{h}, u, t) = \mathrm{Cov}\big(Y(\mathbf{x}, t), Y(\mathbf{x}-\mathbf{h}, t-u)\big)$$

A continuous, bounded, symmetric and integrable function $c(\mathbf{h}, u, t)$ is a covariance function if and only if

$$c_{\boldsymbol{\omega}}^{\mathcal{F}}(u, t) = \int \exp(-\imath \mathbf{h}^{\mathsf{T}} \boldsymbol{\omega}) c(\mathbf{h}, u, t)\, \mathrm{d}\mathbf{h}$$

is a covariance function for almost all $\boldsymbol{\omega} \in \mathbb{R}^d$.

> We are looking for covariance functions $c_{\boldsymbol{\omega}}^{\mathcal{F}}(\cdot,\cdot)$ whose Fourier transform exists.

Example

Initial covariogram:

$$c_{\boldsymbol{\omega}}^{\mathcal{F}}(u, t) = \exp\big(-\frac{a_1}{4}\|\boldsymbol{\omega}\|^2\big) \exp\big(-\frac{a_2}{4}(\|\boldsymbol{\omega}\|^2 + a_3)u^2\big) \exp\big(-\frac{a_4}{4}(\|\boldsymbol{\omega}\|^2 + a_5)t^2\big)$$

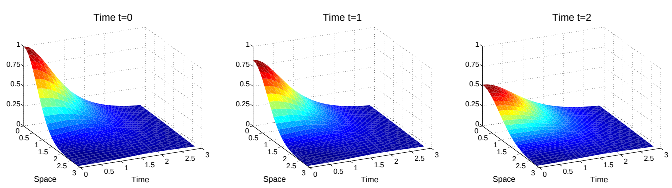
Resulting six-parameter spatio-temporal isotropic covariogram:

$$c^{\circ}(h, u, t, \boldsymbol{\theta}) = \frac{\theta_1}{(1+\theta_3^2 u^2 + \theta_4^2 t^2)^{d/2}} \exp\Big(-\frac{\theta_2^2 h^2}{1+\theta_3^2 u^2 + \theta_4^2 t^2} - \theta_5^2 u^2 - \theta_6^2 t^2\Big)$$

Associated spatio-temporal isotropic variogram:

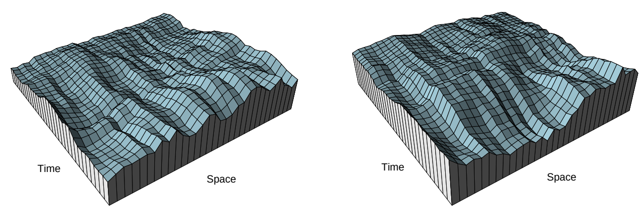
$$2\gamma(h, u, t, \boldsymbol{\theta}) = 2c^{\circ}(0, 0, t, \boldsymbol{\theta}) - 2c^{\circ}(h, u, t, \boldsymbol{\theta})$$

Surface Plots



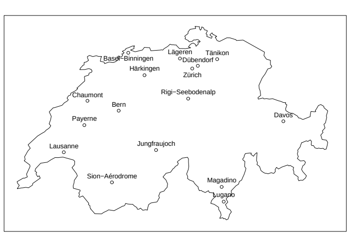
$c^{\circ}(h, u, t, \boldsymbol{\theta})$ with $\boldsymbol{\theta} = (1, 1, 1, 0.4, 0.4, 0.2)^{\mathsf{T}}$

Realizations



$c^{\circ}(h, u, t, \boldsymbol{\theta})$ with $\boldsymbol{\theta} = (1, 1, 1, 0.4, 0.4, 0.2)^{\mathsf{T}}$

Application: Ozone Data



- 16 'National Air Pollution Monitoring Network' stations in Switzerland
- Ozone level is automatically measured in μg/m^3 every half hour
- Aggregated daily data beginning with March 1999 for a period of 7 weeks

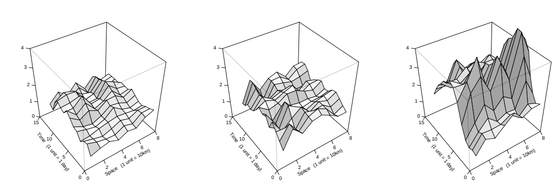
Empirical Spatio-Temporal Variograms

$$\gamma(h, u, t, \boldsymbol{\theta}) = \begin{cases} 0 & \text{if } h = 0 \\ \theta_7 + \theta_1\Big(1 - \dfrac{1}{1+\theta_3{}^2 u^2 + \theta_4{}^2 t^2} \\ \quad \times \exp\Big(-\dfrac{\theta_2{}^2 h^2}{1+\theta_3{}^2 u^2 + \theta_4{}^2 t^2} + \theta_5{}^2 u^2 + \theta_6{}^2 t^2\Big)\Big) & \text{otherwise} \end{cases}$$

estimated with

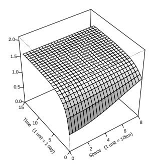
$$\hat{\gamma}(h_k, u, t_r) = \frac{1}{2\,\mathrm{card}\{J\}} \sum_{(i,j,r,s)\in J} \big(Y(\mathbf{x}_i, t_r) - Y(\mathbf{x}_j, t_s)\big)^2$$

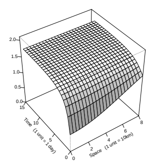
$$J = \big\{(i, j, r, s) : \|\mathbf{x}_i - \mathbf{x}_j\| \in [h_k - 7.5\text{km}, h_k + 7.5\text{km}], t_r - t_s = u\big\}$$

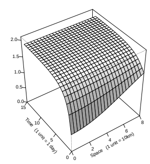


Fitted Spatio-Temporal Variograms

	Model I	Model II	Model III
θ_1	0.543	1.056	1.091
θ_2	0.146	0.127	0.123
θ_3	—	0.938	0.177
θ_4	—	—	0.000
θ_5	—	—	1.683
θ_6	—	—	0.027
θ_7	1.485	0.609	0.611
RSS	1.375	1.210	1.197







Conclusion and Outlook

- Methodological and ‘philosophical’
- Local variogram estimation
- Improve the minimization procedure
- Simulation with spectral methods
- Apply to other datasets
- State-space decompositions

References

Bochner (1933). Monotone Funktionen, Stieltjessche Integrale und harmonische Analyse. *Mathematische Annalen*, **108**, 377–410.

Cressie and Huang (1999, 2001). Classes of nonseparable, spatio-temporal stationary covariance functions. *Journal of the American Statistical Association*, **94**, 1330–1340; **96**, 784.

Dubois (2000). *Intégration de Systèmes d'Informations Géographiques (SIG) et de méthodes géostatistiques. Applications à la cartographie de pollutions radioactives dans l'environnement*. PhD dissertation, Université de Lausanne.

Genton and Furrer (1998a). Analysis of rainfall data by robust spatial statistics using S+SpatialStats. *Journal of Geographic Information and Decision Analysis*, **2**, 126–136.

Genton and Furrer (1998b). Analysis of rainfall data by simple good sense: Is spatial statistics worth the trouble? *Journal of Geographic Information and Decision Analysis*, **2**, 11–17.

Gneiting (2001). Nonseparable, stationary covariance functions for space-time data. Technical Report 63, NRCSE.