Time-series analyis Space-time geostatistics

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Outline

- Concepts of space and time
- Space-time processes
- Time-series analysis
 - Single time-series
 - Time-series modelling: AR models
 - Time-series modelling: spectral analysis
 - Time-series modelling: PCA
 - Multiple time-series
- Spatial analysis
- Spatio-temporal kriging
- Empirical Orthogonal Functions
- Spatio-temporal point patterns
- Conclusion



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Topic: Concepts of space and time

- space
- 2 time
- space and time

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Space

- Refers to processes that occur in space (1D, 2D, 3D)
- Often there is spatial dependency
 - "nearby" locations have more similar attributes than "far away"
- 2D or 3D dependency may be **isotropic** (same in all directions) or **anisotropic** (stronger in one direction)
- Anisotropic dependency is **symmetric**: the same "forward" or "backward" in each 1D
 - ▶ e.g., main axis of long-range 2D dependence 30° (NNE) is the same as 30° + 180° = 210° (SSW)
- This is captured in the definition of spatial autocorrelation
 - differences are squared; there is no "head" or "tail" of a point pair

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Time

- Refers to processes that occur in time
- Usually there is temporal dependency
 - attribute values do not change (completely) randomly over time
 - they evolve, and closely-spaced events have similar values
- Time is 1D and asymmetric because time only flows in one direction
 - It is a deep philosophical question as to why, but it is a consistent observation
 - So, "forward" and "backward" cross-dependencies may be different
 - ► However, "forward" and "backward" auto-dependencies are identical

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- Refers to processes which occur in both space and time
- There may be either or both spatial and temporal dependence
- These may be independent or not

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time stamp a moment in time, to some resolution snapshot the state of nature at one moment in time interval time between two snapshots linear a series of moments cyclical time considered as a repeating cycle discrete separate moments in time continuous moments in time follow each other continuously instantaneous measured directly at one point in time

- e.g., air T, ground-water depth
- e.g., location of an observation

interval directly measured over some known interval

• e.g. stream flow; mean air T using an integrating recorder

cumulative measured at one time from an accumulation over timee.g., daily rainfall from an accumulating rain gauge

Temporal aggregation

- Upscaling by a representative time
 - e.g., minimum daily T from a single measurement at 0500
- Upscaling by aggregation
 - e.g., monthly GDD from daily GDD
- How to aggregate?
 - sum (cumulative)
 - mean, median ... (central tendency)
 - min, max . . . (extremes or quantiles)
 - ▶ ...

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Outline

Concepts of space and time

Space-time processes

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All processes occur over some time period (long or short); many processes take place in geographic space.

Space-time processes may be viewed as:

- **9** spatial only: time is not important
 - consider at one "instant" (conceptually 0-dimensional time)
 - reduce to one temporal point by a summary statistic (average, maximum ...)
- 2 temporal only: space is not important
- **§** spatio-temporal: space and time must both be considered

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processes dynamic, cause effects at locations in space

• e.g., atmospheric processes cause weather

variables what is observed at defined coördinates in space and/or time

- e.g., measured temperature, barometric pressure, precipitation . . .
- measurements referred to a specific time may be "instantaneous", time-averaged, or cumulative

A taxonomy of space-time processes (1)

• Purely **spatial**

- observations all refer to one time or time period
 - represented by a single time stamp, which can represent any length of time
- this can be an aggregate time, e.g., average or cumulative over some time period
- any difference in time of observation is considered unimportant ("nothing" has changed in the intervening time)
 - ★ or, temporal differences are negligibly small compared to spatial differences

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A taxonomy of space-time processes (2)

Purely temporal

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- observations all refer to "one" location
 - ★ represented as a point or "homogeneous" area
- this can be an aggregate location, e.g., average of a set of weather stations
- spatial differences (e.g., small offsets) are negligible
 - ★ or, spatial differences are negligibly small compared to temporal differences
- or we only care about the spatial area as a unit

• Spatio-temporal

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- observations have both a location and a time stamp
- observations at different locations may have been made at different times
- or there may be the same time-series of observations at each location
- space and/or time may be aggregates

Example of space-time processes: Soil organic carbon (SOC) 1 – purely spatial

• soil samples in an agricultural field, all collected at the "same" time

- time differences in sampling are insignificant compared to process time (e.g., SOC decomposition)
- aim is to map SOC distribution in the field and relate to other soil or land properties
- soil samples in a forest, collected over a number of years
 - aim is to assess SOC stocks in the area
 - must assume no drivers of SOC change in this time, no seasonal effects
 or at least these are negligibly small compared to spatial variation
 - must justify this assumption from literature or small time-series studies

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- **Repeat** soil samples at **one** location before and after manure and fertilizer applications, crop growth, crop harvest, residue incorporation, winter weather ...
 - Aim is to reveal SOC dynamics as influenced by weather and management
 - Since soil sampling is inherently destructive it is impossible to sample repeatedly at the same exact location
 - If using close-by locations micro-scale spatial variation and small support will cause problems.
 - ★ Solution: use composite sampling from the one location (i.e., support of several tens of m²)

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- Repeat samples at multiple sites in an agricultural field
 - Aim is to discover if there are different temporal dynamics at different locations
 - Can also map more efficiently (more information), and produce maps for different times
 - May relate to spatio-temporal covariables (e.g., weather)

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USA unemployment rate - spatial

Unemployment rates by county, August 2011 - July 2012 averages (U.S. rate = 8.4 percent) % and over % to 13.9% % to 11.9% 0% to 9.9% 0% to 7.9% 4.0% to 5.9% SOURCE: Bureau of Labor Statistics Local Area Linemrinement Statistics 3.9% or lower

source:

http://moneybasicsradio.com/2012/09/us-unemployment-rate-by-county/

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USA unemployment rate – temporal



Source: Federal Reserve Bank of Dallas, LAUS.

source:

https://www.austinchamber.com/blog/03-14-2017-job-growth-unemployment

USA unemployment rate – spatio-temporal

source: https://www.huffingtonpost.com/2014/08/31/
america-unemployment-map_n_5744656.html

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- Time-series of unemployment; could examine each county's time series separately
- **2** Spatial dependence at each time slice
- Spatio-temporal interaction: The spatial pattern is not the same at each time slice

A taxonomy of spatio-temporal analysis

Following the taxonomy of processes, how do we analyze them?

- **9** spatial at each time slice, independently
 - > point geostatistics, point-pattern analysis, spatial autoregressive models
- 2 temporal at each location, independently
 - time-series analysis [9]; see next slide
- spatial at each time slice, but using a temporally-pooled estimate of spatial dependence
 - spatial statistics as (1) but each time of observation is considered a replication of the spatial dependence
- spatio-temporal as a combined model
 - both spatial and temporal statistics

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Topic: Time-series analysis

Only considering time:

- **(**) a series of observations over time at **one location**
 - single time series
 - one variable measured at different times
 - multiple (also called "multivariate") time series
 - \star several variables, measured together at the same observation times

same, at multiple locations

- single or multiple time series at each location
- but with no explicit spatial dimension
 - ★ no coördinates, no distance
 - ★ so it is not geostatistical
- a type of multiple time series: attribute is the same but at different (non-georeferenced) locations

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A series of readings of the **same** variable at the **same** location, at **different** times

- Often at regular intervals (15-min, hourly, daily, ...)
- But can be at irregular times, although analysis becomes much harder

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Components of a single time-series

Up to six components *may* be present:

trend the variable changes systematically with time

• e.g., increasing daily mean T

periodic the variable **fluctuates** around a central value, with a fixed period

• e.g., hourly T over a day; daily T over a year

cyclic but non-periodic the **fluctuates** around a central value, with a variable period

• e.g., predator-prey abundances

anomalies unusual values of the variable that do not fit a pattern ("spikes")

 $\bullet\,$ e.g., daily T during an unusual weather event

correlated noise "small" variations after accounting for the above, with temporal dependence

white noise uncorrelated "small" variations

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How to identify, separate and quantify these?

- decomposition
- 2 autocorrelation analysis
- Modelling

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Example: Groundwater level: time series





Monthly 1975-2005; irrigation well in Anatolia (Turkey)

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Time series as bar graph



Monthly 1975-2005; irrigation well in Anatolia (Turkey)

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Time-series analysis -(1) decomposition

- Decomposition: identify the components of the series
 identify and remove periodic component
 - * single amplitude or moving amplitude, user-specified "span"
 2 fit a trend to the non-periodic component by local polynomial regression ("Locally-weighted scatterplot smoother" = "lowess")
 - * user-specified "span" (smoothing window) to degree of smoothing
 - **(3)** the residual "noise" = **anomalies** from trend and cycles
- These components should correspond to **processes** that produced the time series

Groundwater level: decomposition (1)



Trend modelled with a moving window

Yearly cycle assumed the same - does this seem correct?

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Groundwater level: decomposition (2)



Magnitude of yearly cycle increases with time - reduces remainder

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Groundwater level: decomposition (3)



Anatolia well 1, decomposition

Trend and remainder after subtracting trend (note absolute values) Note large anomaly in 1988

Interpretation of time-series decomposition

- Aim: understand the underlying process that produced the time-series
 - Example: daily T cycle driven by insolation (clue: the cycle is 24 hours!)
- Aim: determine the magnitude of changes (trend) or persistence of phenomena (anomalies)
 - and from that, infer causes
Interpretation: groundwater example (1)

- Groundwater was closer to the surface from 1975–1980 and then began a steady **trend** to become deeper
 - Increased groundwater extraction for irrigation? Decreased winter rainfall for recharge?
- There is a **yearly cycle**
 - explained by extraction for irrigation (summer) and recharge from rainfall and irrigation excess (winter)
- This cycle seems to be getting stronger
 - suggesting increasing irrigation demand
- A strong **anomaly** of draw-down and then recharge was observed for 1988 why?
- Residual noise may have temporal autocorrelation see next slides

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- Auto-correlation analysis: time dependence of observations
 - of the original series
 - after de-trending and/or removing any cycles (i.e., after decomposition)
- Question: how strongly are observations linked in time?
- Question: how long does this autocorrelation last ("range")?

Serial autocorrelation

If the random process that generated the time series is 2^{nd} order stationary (mean and variance are constant over time), at lag k the autocorrelation is:

$$\rho_k = \frac{E\left[(z_t - \mu)(z_{t+k} - \mu)\right]}{\sigma_z^2} \tag{1}$$

 ρ_k can be estimated as r_k :

$$r_{k} = c_{k}/c_{0}$$
(2)

$$c_{k} = \frac{1}{N} \sum_{t=1}^{N-k} (z_{t} - \bar{z})(z_{t+k} - \bar{z}), k = 0, 1, 2...K,$$
(3)

$$var[r_{k}] \approx \frac{1}{N} \left(1 + 2\sum_{\nu=1}^{q} r_{q}^{2} \right), k > q$$
(4)

- Original series: assume first- and second-order stationarity
- **Remainder** series (after subtracting a trend): only assume constant variance and co-variance for all lags
- Use the approximate formula for variance (previous slide) to establish confidence limits: is the observed correlation at a given lag significantly non-zero?

Groundwater level: autocorrelation - original series



Lag 1 is one year Autocorrelation increases exactly on the year, but less each year

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Groundwater level: autocorrelation - remainders



No autocorrelation at one year; negative at two years!

Artefact of moving average?

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Interpretation: groundwater example (2)

- Original time series shows strong positive autocorrelation
 - decreases over a year, but then increases a bit on the yearly cycle
 - \blacktriangleright steadily decreases over the years, but still $\rho \approx$ 0.5 after five years
- Residual noise is positively autocorrelated for one year
 - this reflects continuity month-to-month

Partial autocorrelation

- Autocorrelation after accounting for previous lags; symbol φ_{k,j}: coefficient j of an autoregressive process of order k
- Example: if all autocorrelation can be explained at lag 1, then there is no partial autocorrelation at lags 2, 3, ..., so that the apparent autocorrelation at these lags can be explained by repeated lag-1 correlations

$$\mathbf{P}_{\mathbf{k}}\phi_{\mathbf{k}} = \rho_{\mathbf{k}}$$

$$\mathbf{P}_{\mathbf{k}} = \begin{bmatrix}
1 & \rho_{1} & \rho_{2} & \cdots & \rho_{k-1} \\
\rho_{1} & 1 & \rho_{1} & \cdots & \rho_{k-2} \\
\vdots & \vdots & \ddots & \ddots & \vdots \\
\rho_{k-1} & \rho_{k-2} & \rho_{k-3} & \cdots & 1
\end{bmatrix}$$

$$\rho_{j} = \phi_{k,1}\rho_{j-1} + \cdots + \phi_{k,k}\rho_{j-k}, \ j = 1, 2, \dots k$$
(5)
(6)
(7)

Groundwater level: partial autocorrelation



Partial autocorrelation, Anatolia well 1

Lag 1 month strongly positive Lag 2 slightly negative after accounting for lag 1 Lag 4–8 (half-season), 12 (?), 13 (full season) significant

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Time-series modelling: AR, MA, ARMA, ARIMA

- Aim: a mathematical description of the series
 - Generally used for forecasting
 - assuming that the statistical characteristics of the time-dependent process are the same in the future as in the past
 - Also can be used to understand the process from the form of the best-fitted model
 - Also can be used for **gap filling** of incomplete series
- Model types: AR (auto-regressive), MA (moving average), ARMA, ARIMA
 - ► I = "integrated", for the degree of differencing applied to the series before ARMA)
- See Shumway and Stoffer [9], Wilks [11, Ch. 9], Box [1]

Autoregressive models (AR)

- Current value of a process is expressed as a finite and linear sum of previous values of the process
- this is the temporally autocorrelated noise

$$\tilde{z}_t = \phi_1 \tilde{z}_{t-1} + \phi_2 \tilde{z}_{t-2} + \dots + \phi_p \tilde{z}_{t-p} + a_t \tag{8}$$

- ϕ_i are the autocorrelation parameters (strength of dependence at each lag)
- a_t is the white noise, sometimes called "shock" at time t
- simplest is AR(1): $\tilde{z}_t = \phi_1 \tilde{z}_{t-1} + a_t$: dependence only on previous value

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Time-series modelling: spectral analysis

- Fourier (1807): any *second-order stationary* time-series can be **decomposed** into **sums of sines and cosines** with increasing **frequencies**, each of varying **amplitude** or "power"
 - trend removed and auto-covariance not dependent on position in the series

• Frequency ω : the number of divisions of one cycle per unit time

- \blacktriangleright e.g., a one-year cycle (as in the groundwater levels), $\omega=12$ is a monthly frequency
- By the Nyquist-Shannon sampling theorem, a function is completely determined by sampling at a rate of $1/2\omega$
- ► a time-series with n samples per cycle → can estimate spectral densities for n/2 frequencies.
- **Period** *T*: inverse of frequency: number of divisions required for one full cycle; $T = (1/\omega)$

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- Reveals the relative strength of the frequencies of periodic time series
 - Examples: sunspot intensity; El Niño/La Niña cycles vs. annual cycles
- Usually applied after **de-trending** that is a separate feature of the time-series.

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Spectral decomposition

Covariance sequence γ_t decomposed into spectral densities f:

$$\gamma_t = rac{1}{2\pi} \int_{-1/2}^{+1/2} e^{2\pi i \omega_f t} f(2\pi \omega_f) d\omega_f$$

where ω_f is the frequency (cycles per unit of time).

Recall: $e^{ix} = \cos x + i \sin x$

This can be inverted to give the density at each frequency:

$$f(\omega) = \gamma_0 \left[1 + 2\sum_{i}^{\infty} \rho_t \cos(\omega t) \right]$$

where γ_0 is the overall covariance.

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Spectral analysis as a linear regression problem

Time series of length n, gives (n-1) predictors $a_0 \ldots a_{n/2}, b_1 \ldots b_{n/2-1}$ of the response variable:

$$x_t = a_0 + \sum_{k=1}^{n/2-1} \left[a_k \cos(2\pi kt/n) + b_k \sin(2\pi kt/n) \right] + a_{n/2} \cos(\pi t)$$

Note how at each value of k in the sum the frequency is increased.

 a_0 is the intercept, it centres the series around its mean \overline{x} .

The highest frequency is $\omega = 0.5$ cycles per sampling interval, the lowest is $\omega = 2\pi$, i.e., one cycle.

(Note: the computation is usually with the Fast Fourier Transform).

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The periodogram

This is used to estimate the spectral density (R spectrum function)

The periodogram at a given frequency ω : the squared correlation between the time series X and the sine/cosine waves at that frequency:

$$I(\omega) = \frac{1}{n} \left| \sum_{t} e^{-i\omega t} X_t \right|^2 = a_k^2 + b_k^2$$

- The spectrum is scaled by $1/\omega$, i.e. the inverse of the frequency.
- ullet So the spectral density is computed over $-\omega/2\ldots+\omega/2$
- Since the function is symmetric, it is displayed for $0 \ldots + \omega/2$.
- Groundwater example: $\omega = 12$; the decomposition is from $0 \dots \omega/2 = 6$ periods per cycle.
- One period per cycle is annual, 2 per cycle is semi-annual, 6 periods is bi-monthly, etc.

- The time-series is usually noisy; we want to reveal the various periodicities w/o the noise
- So, smooth the series with **Daniell windows**, trial-and-error spans m
 - each spectral density estimate is computed as the mean of the m/2 preceding and following periodogram values

Example periodogram – log scale



Series: x Smoothed Periodogram

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Phase

- The series can also be expressed as a sum of cosines, each term with a **phase**: i.e., a lag from $\phi_k \in [-\pi/2 \dots 3\pi/2]$
- The phase angle $\phi_k = \tan^{-1}(b_k/a_k)$
- Then $f(t) = \frac{1}{2}a_0 + \sum_{k=1}^n \sqrt{a_k^2 + b_k^2} \cos\left(\frac{2\pi nt}{\omega} \phi_k\right)$
- The phase angle gives the offset from the centre of the period
- Reference: Jakubauskas, M. E., Legates, D. R., & Kastens, J. H. (2001). *Harmonic analysis of time-series AVHRR NDVI data*. photogrammetric Engineering and Remote Sensing, 67(4), 461–470.

Time-series modelling: PCA

- Principal Components Analysis (PCA): convert a number of inputs into the same number of outputs
 - Often applied to time-series of images
 - orthogonal i.e., uncorrelated
 - in descending order of variance explained importance of each component
 - contribution of each original image to each synthetic image
- Reveals correlation among dates, separates overall value (first component) from contrasts between dates
- If there are **periods** this should come out in one or more components
- Can also find anomalies not explained by any overall value or periods

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What does PCA do?

- The vector space made up of the original variables is projected onto another space;
- The new space has the same dimensionality as the original¹, i.e., there are as many variables in the new space as in the old;
- In this space the new synthetic variables, also called principal components are orthogonal to each other, i.e. completely uncorrelated;
- The synthetic variables are arranged in decreasing order of variance explained; and the total variance is unchanged;
- The contribution of each original variable to each synthetic variables is given;
- Seach observation can be **re-projected** into the new (PC) space.

¹unless the original was rank-deficient

Mathematics: Eigen decomposition

The key insight is that the **Eigen decomposition**² of the covariance or correlation matrix **C** orders the synthetic variables into descending amounts of variance, and ensures they are **orthogonal** (Hotelling 1933).

- Decompose a square, symmetric positive-definite matrix, e.g., the correlation matrix C formed from a data matrix such that $AC = \lambda C$
- Eigenvalues: a diagonal matrix λ; off-diagonals 0, i.e., no covariances, so orthogonal
- Eigenvectors: the transformation matrix **A**, a coördinate transformation such that the matrix multiplied by the diagonal eigenvalues matrix is the same as multiplication by a matrix made up of the eigenvectors
- Eigenvectors span an orthogonal **vector space** onto which we can **project** the original data.

²(German *eigen* \approx English "own, belonging to oneself") $\Rightarrow (a) + (a$

Computation

- $|\mathbf{C} \lambda \mathbf{I}| = 0$: a determinant to find the **eigenvalues** of the correlation matrix
 - these are sometimes called the characteristic values
 - their relative magnitude is the proportion of the original covariance explained
- Then the axes of the new space, the eigenvectors γ_j (one per dimension) are the solutions to (C λ_jI)γ_j = 0
- Obtain **synthetic variables** by projection: **Y** = **PC** where **P** is the row-wise matrix of eigenvectors (rotations).

Example: Time series of diurnal temperature differences

- 中国江苏沛县 Pei county in JiangSu province, PRC
- MODIS³ daily land-surface temperature product⁴
- Images are diurnal temperature differences (day night) between two MODIS products, units are Δ°C
- 30 Oct 03 Nov 2000 (Julian days 304 ff.); Soil is drying after a heavy rain
- Objective: try to relate DTD to soil texture and organic matter
- Reference: Zhao, M.-S., Rossiter, D. G., Li, D.-C., Zhao, Y.-G., Liu, F., & Zhang, G.-L. (2014). Mapping soil organic matter in low-relief areas based on land surface diurnal temperature difference and a vegetation index. Ecological Indicators, 39, 120–133.⁵

⁴available at http://ladsweb.nascom.nasa.gov/data/search.html ⁵http://doi.org/10.1016/j.ecolind.2013.12.015

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³http://modis.gsfc.nasa.gov

Original images



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> summary(pca)
Importance of components:

 PC1
 PC2
 PC3
 PC4

 Standard deviation
 1.8232
 0.40406
 0.3230
 0.20810

 Proportion of Variance
 0.9145
 0.04492
 0.0287
 0.01191

 Cumulative Proportion
 0.9145
 0.95938
 0.9881
 1.00000

The four DTD images are highly-correlated, 92% of the information is in common, i.e., over the four days the same areas tend to have narrow and wide DTD ranges

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PCA results - loadings

Contributions of each original image to each synthetic image

> pc\$rotation PC1 PC2 PC3 PC4 DTD304 -0.4447 0.5893 0.5870 0.3322 DTD306 -0.6084 0.3379 -0.5200 -0.4952 DTD307 -0.4717 -0.3857 -0.3677 0.7025 DTD308 -0.4578 -0.6243 0.4998 -0.3884

PC1 "intensity" of the phenomenon over all days

PC2 contrast between first two and second two days *after* accounting for the mutual correlation of PC1

PC3 contrast between middle two and end two days after ...

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Biplots

These show positions of the observations as synthetic variables (bottom, left axes) and the correlations/variances of the original standardized images (top, right axes):



First PC is **overall intensity** across all 4 dates; other PCs show **contrasts** between dates

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PCs (synthetic bands) - same stretch



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PCs (synthetic bands) – individual stretch

1830000

120000



PC3

y 1830000 384000

3820000



This allows to visualize contrasts within a PC

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495000 500000

480000 485000 490000

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480000 485000 490000 495000 500000 x

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Groundbreaking paper, 200+ citations:

Eastman, J., & Fulk, M. (1993). Long Sequence Time-Series Evaluation Using Standardized Principal Components (reprinted from Photogrammetric Engineering and Remote-Sensing, Vol 59, Pg 991–996, 1993). Photogrammetric Engineering and Remote Sensing, 59(8), 1307–1312.

- Sensor was AVHRR
- Images were monthly maximum NDVI, 1986-1988 (three full years)

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Synthetic images

Standardized Principal Components of Monthly NDVI Images, Jan. 1986 - Dec. 1988



Green = "+" score, Red = "-"

Sign is arbitrary, here chosen to show high NDVI in green.

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Loadings



PC1 All bands contribute pprox equally:(overall intensity)

PC2 shows annual movement of Intertropical Convergence Zone

PC3/4 show deviations from PC2 seasonality

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Interpretation

Synthetic bands images summarizing all original images, according to the PCs

- Loadings relation between original images (dates, x-axis) and contribution to the PC (y-axis).
 - Note decreased absolute loadings at higher PCs, this is because they represent less of the total variability of the 36 images
- PC1: \approx equal contribution of all dates (overall vegetation vigour averaged over the 3 years)
- PC2: + correlation in N. hemisphere summer, in winter (seasonality) – Intertropical Convergence Zone
- PC3/4: deviations from PC2 seasonality note time lag of greening/senescence
- PC5: detecting sensor drift

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- Time-series of several variables measured at the same times
 - \blacktriangleright e.g., T, relative humidity, precipitation . . . at a single weather station
- These may be cross-correlated at various lags
- In spectral analysis, this is reflected as their **coherency** (correlation at a given period) and **phase difference** (coherent but offset)

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Groundwater level: two wells

Anatolia, two wells



Clearly they are related - but at what lags? and how closely?

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Groundwater level: cross-correlation

Cross-correlation, Anatolia well 1 vs. well 2



May be **asymmetric** – one station may be "ahead of" the other Here highest cross-correlation is at +4 months, well 1 leads well 2

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Groundwater level: cross-spectral analysis



Well 1 "leads" well 2 at some periods

Clear phase differences and loss of coherence.

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Time-series analysis: computing

- CRAN Task View
 - cran.r-project.org/web/views/TimeSeries.html
- base R has many functions, class ts for time-series objects
 - decomposition stl
 - autocorrelation acf, pacf
 - modelling ar, arima
 - spectral decomposition (Fourier analysis) spectrum
- specialized packages for advanced analysis
- R tutorial "Time series analysis in R" http://www.css.cornell. edu/faculty/dgr2/pubs/list.html#pubs_m_R

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Outline

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- Space-time processes
- Time-series analysis
 - Single time-series
 - Time-series modelling: AR models
 - Time-series modelling: spectral analysis
 - Time-series modelling: PCA
 - Multiple time-series
- 4 Spatial analysis
 - Spatio-temporal kriging
 - Empirical Orthogonal Functions
 - Spatio-temporal point patterns
- Conclusion
- References

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This has been covered in other lectures; included here just to emphasize that at one time slice there is usually some spatial structure.

- trend surfaces
- elation to other spatially-distributed attributes
- Iocal spatial dependence, also after accounting for (1) and (2)

- TSA uses the correlation function, geostats the the variogram to examine auto-dependence
 - for second-order stationary series there is a direct conversion
- TSA uses autoregressive moving-average (ARMA) models to describe the time-evolution of a process
 - however there are also 2D spatial ARMA processes using the von Neumann neighbourhood (a diamond-shaped neighbourhood that defines a set of grid cells)

Example of spatial structure



PM10 on 2009-03-21

Particulate matter (PM10, μ g m⁻³) at stations in Germany, one date; shows regional trend and residual local spatial dependence

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From the EU⁶:

- 50 $\,\mu{\rm g}$ m^-3 over any single 24-hour period; can be exceeded 35 times per year
- 40 $\,\mu\mathrm{g}\,\,\mathrm{m}^{-3}$ averaged over a year

Previous slide shows all (rural) stations below the one-day threshold on 2009-03-31.

⁶http://ec.europa.eu/environment/air/quality/standards.htm = = = = D G Rossiter (CU) Time-series analyisSpace-time geostatistics April 23, 2018 80 / 131

Spatial variograms



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Ordinary Kriging predictions



35 30 25 20 lumped variogram model

PM10 on 2009-03-21

one date variogram model

lumped, 200 days variogram model

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Ordinary Kriging onto the centres of 0.25°x 0.25°grid cells.

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Topic: Spatio-temporal kriging

- Both space and time drive the observed process
- These may be independent or interacting
- Observations have both a location and time stamp
 - various ways to organize, see next slide
 - special data structures are required
- We can compute spatio-temporal empirical variograms;
 - These can be modelled with authorized variogram models
 - The fitted models can be used to interpolate in space and time by kriging
- Examples using R package gstat, many other applicable packages
 - CRAN Task View https://cran.r-project.org/web/views/SpatioTemporal.html

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Organization of space-time data



Source: Pebesma [8]

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- grid: all combinations have been observed
- sparse grid: regular lattice but some missing
- **irregular**: each observation has its own time stamp and location
- trajectory: individual can move in both space and time
 - e.g., animals with tracking collars

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Space-time dependence

The value in **s**pace and *t*ime of some target variable Z can be expressed as:

$$Z(\mathbf{s},t) = Z^*(\mathbf{s},t) + \varepsilon'(\mathbf{s},t) + \varepsilon(\mathbf{s},t)$$
(9)

- s: spatial vector (commonly 2D); t: time
 - Z* is the deterministic, also called "structural" or "trend" component in both space and time
 - This can be modelled physically (e.g., process model) or empirically (e.g., regression on coördinates or covariates)
 - ε' is a spatio-temporally correlated space-time process of the residuals
 - ε is pure noise; it assumed to be purely random ("white noise")

Ignoring any trend in space and time, Z^* becomes a constant mean in both space and time:

$$Z(\mathbf{s},t) = \mu + \varepsilon'(\mathbf{s},t) + \varepsilon(\mathbf{s},t)$$
(10)

There is no way to objectively decide if there is a structural component, or if present, how to model it.

In practice local approaches can be used even if there is a structure; we lose information but the predictions may be satisfactory.

Location of PM10 monitoring stations in NRW (D)



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Direct & cross-correlations, PM10, NRW



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- Each station has temporal dependence: one day's PM10 is "similar to" the next, to some lag \rightarrow a somewhat persistent atmospheric phenomenon
- Stations can be cross-correlated to others at time lag 0 (i.e., spatial correlation) we can see if this depends on distance or a trend
- Stations can also be cross-correlated at different time lags, and this may be asymmetric
 - e.g., station A may lag behind station B, for example process could be wind blowing PM10 from B to A

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Spatio-temporal variograms

- Compute semi-variance at combined lags
 - h spatial lag, usually 2D, can include a direction (anisotropy)
 - u temporal lag, 1D
- At all combinations of space and time:

$$\gamma(\mathbf{h}, u) = \frac{1}{2} \sum (z_{\mathbf{s},t} - z_{\mathbf{s}+\mathbf{h},t+u})^2$$
(11)

- Summarized in lags (bins) to have enough point-pairs
- Isotropic in 2D space \rightarrow 2D variogram (isotropic spatial + temporal separations)
- Anisotropic in 2D space \rightarrow 3D variogram! (anisotropic spatial + temporal separation)

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Spatio-temporal variograms – view 1



PM10 concentrations, one spatial variogram per temporal lag

Spatio-temporal variograms – view 2



Semivariance, PM10

PM10 concentrations, distance/time lag matrix

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Spatio-temporal variograms - view 3



PM10 concentrations, distance/time lag matrix, wireframe The two **marginal** (space and time) variograms have **different sills**

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Explanation

- Zonal anisotropy: different sills in the two dimensions
- Variograms are erratic because of few stations
- Time and space lag 0 **marginal** variograms show typical empirical variogram (exponential model)?
- Marginal total sill for space is about half that for time
 - ▶ i.e., more time than space variability in PM10 over Germany
- As temporal lags increase:
 - spatial dependence becomes less (shorter range; higher nugget/sill ratio)
 - total variability (total sill) increases
- Interesting anomaly at longer time lags, 25 km separation wind?

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Spatio-temporal combined model - viewpoints

time as an extra dimension equivalent to space

- this is called the "metric" model
- time asymmetry can not be modelled
- time must be re-scaled with the space-time anisotropy ratio to match space
- spatial and temporal dependence structure must be the same
- rarely realistic
- eparate covariance structures for space and time
 - this is called the "separable covariance" model
 - no interaction between space and time
- interacting covariance structures for space and time
 - this is called the "sum-metric" model
 - a metric model plus a purely spatial and also a purely temporal component added to it

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Modelling space-time variograms

Models forms, with their assumptions:

metric time is equivalent to an additional "spatial" dimension, re-scaled to match the spatial units

- single model form, nugget and partial sill
- unrealistic if sills in space vs. time not the same

separable time and space are modelled separately, each in their own units; the variogram is a proportional product

- structure of temporal variation must be the same at all locations
- structure of spatial variation must not vary over time
- not realistic in most contexts

sum-metric also has a space-time term, allowing for interaction

Metric covariance structure

$$C(h, u) = C\left(\sqrt{h^2 + (\alpha u)^2}\right)$$
(12)

- One covariance structure C
- h is the distance lag, generally 2D
- *u* is the time lag, here another "dimension"
- α is a scaling factor ("metric") to match spatial and temporal units: the **space-time anisotropy ratio**

This represents **geometric anisotropy**, i.e., same structure, nugget and partial sill but the range varies in different dimensions (here, the time vs. space dimensions)

e.g., $\alpha = 20 \ km \ d^{-1}$ means that a lag of 20 km in space is equivalent to a lag of 1 day in time.

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$$C(h, u) = C_s(h) \cdot C_t(u) \tag{13}$$

- Two covariance structures, one each for space and time
- No interaction; the covariance at a given spatial and temporal lag is just the product of the two marginal covariances
- There is only one joint sill; the two sills of the two components are given as **proportions** of this.

Sum-metric covariance structure

$$C(h,u) = C_s(h) + C_t(u) + C_{st}\left(\sqrt{h^2 + (\alpha u)^2}\right)$$
(14)

• Three covariance structures

- Space, time, and joint each have their own sill, range, and nugget
- *C_{st}* is the metric structure of the residuals, after accounting for space and time separately
- The last term has geometric anisotropy

spatial marginal variogram 3: partial sill, nugget, range temporal marginal variogram 3: partial sill, nugget, range space-time variogram 4: partial sill, nugget, range, **anisotropy**

• The space and time sills have to match, but only for the **residuals** after accounting for the marginal variograms (space and time)

To estimate the three different nuggets it is required to have **repeated** measurements at the same **locations**, as well as **repeated** measurements at the same **times**.

Parameters are fit with fit.StVariogram, which uses the generic optim optimization function.

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Fitted sum-metric variogram – view 1



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Fitted sum-metric variogram - view 2



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Results of space-time kriging



PM10, Germany

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6 Empirical Orthogonal Functions

- Spatio-temporal point patterns
- Conclusion



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Topic: Modelling spatio-temporal structure with EOF

• EOF: Empirical Orthogonal Functions

- mathematically the same as PCA (Principal Component Analysis)
- finds the spatial or temporal patterns of variability of one variable
 - ▶ i.e., spatial patterns over time, or temporal patterns over space
- measures the importance of each contribution
- clusters variables (either time instances or spatial locations) in PC space

Example: Republic of Ireland wind speed

Source: Pebesma [8]



Station locations

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Ireland: time-series at different stations



does not show spatial distances

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Ireland: another space-time plot



does not show spatial distances

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Obvious correlation between stations at each time period

- Low-speed days, e.g., 17-April
- High-speed days, e.g., 20-April
- But sometimes the correlation is lagged: the highest speed at a station comes a day or two after that at another
 - e.g., 21, 20, 19 April
 - Is this from a synoptic event, e.g., Atlantic storm?
- Some temporal dependence, although erratic

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EOF: scree plots



These show the relative importance of each PC The variance is higher in the spatial EOF because many more time replications (two years) vs. space replications (12)

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EOF: biplots



These show the loadings of each variable on the first two PCs (red) and the position of each observation in PC space (black).

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- Aim: analyze point-patterns which may change over time
 - e.g., locations of live trees in a forest plot (some die, some new ones grow)
 - e.g., locations of crime or disease incidences, each with a time stamp
- Q1: Does the structure of the point-pattern change over time?
 - intensity, kernel density, G, F, K, L functions . . .
- Q2: Does the point-pattern at one time affect the pattern at a later time?
 - crossed K function

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Example: time of occurrence



Foot-and-mouth disease, northern Cumbia (England), 2001; from R package stpp, dataset fmd more recent \rightarrow larger symbol; total 648 cases (points) \Rightarrow

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Analysis

Divide into time slices, each with enough cases

- here, 50-day slices (156, 404, 40, 48 cases)
- could also divide by "epidemic stage" from expert opinion
- Oisplay point-pattern in the slice, compute intensity
- Compute point-pattern functions G (closest neighbour), F (empty space), look at pattern over time
- Compute crossed K-function for adjacent time slices, to see if they are independent, attracting, or repulsing
- S From all of this, try to infer mechanisms

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Days 51-100



 $116 \text{ km}^2 \text{ case}^{-1} \text{ solution}$ ics April 23, 2018 118 / 131

G function at each time slice



Strong clustering at each time slice, but amount changes with time

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F function at each time slice



Much more empty space than expected, amount changes with time

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Crossed K function between time slices



0-50 to 51-100: clustered 51-100 to 101-150 \approx independent 101-150 to 151-200 clustered

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- Point-pattern moves over time
- Intensity changes over time
- Nearest-neighbour G function changes over time
- empty-space function F changes over time
 - i.e., distance from an arbitrary position to an occurrence of foot-and-mouth disease
- patterns are *not* independent between the 0-50 and 51-100, and the 101-150 and 151-200 slices
 - in both cases strongly dispersed
 - no interaction between the 51-100 and 101-150 slices

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Further analysis of spatio-temporal point patterns

- " Log-Gaussian Cox Processes"
 - window $W \subset \mathbb{R}^2$, time slice $T \subset \mathbb{R}_{\geq 0}$
 - Cases occur at spatio-temporal positions (x, t) ∈ W × T according to an inhomogeneous spatio-temporal Cox process, i.e., a Poisson process with intensity R(x, t)

i.e., number of cases X_{S,[t1,t2]} is Poisson-distributed conditional on R.
R(s,t) = λ(s)μ(t) exp{Y(s,t)}

▶ i.e., fixed spatial, fixed temporal, and interaction term

• see Taylor et al. [10] (1gcp R package)

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Outline

- Concepts of space and time
- Space-time processes
- Time-series analysis
 - Single time-series
 - Time-series modelling: AR models
 - Time-series modelling: spectral analysis
 - Time-series modelling: PCA
 - Multiple time-series
- 4 Spatial analysis
- Spatio-temporal kriging
- Empirical Orthogonal Functions
- Spatio-temporal point patterns



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- All processes occur in both space and time.
- Unless we restrict to one moment in time or one location in space, or if the variability in one of them is negligible compared to the other, both space and time need to be considered:
 - when modelling the process, and then ...
 - ... interpreting the model to look for causes
- Space and time may be **separable** elements of the analysis, but very commonly the variations in space and time are **not independent**.

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- 5 Spatio-temporal kriging
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- Conclusion



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- Time series: Shumway and Stoffer [9], Wilks [11, Ch. 9], Box [1]
 - these also as e-books via CU library
- Description of R package spacetime: Pebesma [8]
- Spatio-temporal point patterns: Diggle [2], Taylor et al. [10]
- Theory: Kyriakidis and Journel [7], Gneiting et al. [3]
- Applications: Heuvelink and Griffith [5]; Jost et al. [6]; Hengl et al. [4]

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- CRAN Task View: Handling and Analyzing Spatio-Temporal Data: http://cran.r-project.org/web/views/SpatioTemporal.html
- Benedikt Gräler (was in Münster, now at Ruhr University Bochum): http://ben.graeler.org

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