The Periodogram

An approximation to the spectral density of a process observed over a regular $n_1 \times n_2$ lattice is given by the periodogram:

$$I(k_1, k_2) = \frac{1}{4\pi^2} \frac{1}{n_1 n_2} \left| \sum_{s_1, s_2} X(s_1, s_2) \exp\{-i(s_1 k_1 + s_2 k_2)\} \right|^2$$

This is evaluated for frequencies that are multiples of $2\pi/n_1$ and $2\pi/n_2$.

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The empirical covariance function is

$$\hat{C}(h, j) = \frac{1}{n_1 n_2} \sum_{l}^{L} \sum_{m}^{M} (X(l, m) - \overline{X})(X(l + h, m + j) - \overline{X})$$

$l = \max\{1, 1 - h\}, L = \min\{n_1, n_1 - h\}, m = \max\{1, 1 - j\}$ and $M = \min\{n_2, n_2 - j\}$.

It can be shown that

$$I(k_1,k_2) = \frac{1}{4\pi^2}\sum_{h=-n_1+1}^{n_1-1}\sum_{j=-n_2+1}^{n_2-1}\hat{C}(h,j)\exp\{-i(hk_1+jk_2)\}$$

which does not involve any complex arithmetic. Moreover

$$I(k_1,k_2) = \frac{1}{4\pi^2}\sum_{h=-n_1+1}^{n_1-1}\sum_{j=-n_2+1}^{n_2-1}\hat{C}(h,j)\cos\{hk_1+jk_2\}$$

Additional computational saving can be obtained using the fact that $\hat{C}(h,j) = \hat{C}(-h,-j)$.

Properties of the Periodogram

Define

$$s(k) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} C(s) \exp\{-ik's\} ds$$

then

$$2\frac{I(k)}{s(k)} \to \chi^2_2$$

where the limit is taken in distribution. This implies that, asymptotically, $EI(k) = s(k)$ and $\text{var}(I(k)) = s(k)^2$. The former implies that the periodogram is an inconsistent estimator of the spectral density.

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Asymptotically, the ordinates of the periodogram are uncorrelated, so $\mathrm{cov}(I(k_h), I(k_j)) = 0$ if $h \neq j$.

Properties of the Periodogram

The periodogram is biased for finite sample sizes. In fact, in two dimensions,

$$E(I(k)) = \frac{1}{n_1 n_2 (2\pi)^2} \int s(\alpha) W(\alpha - k) d\alpha$$

where

$$W(\alpha) = \frac{\sin^2(n_1\alpha_1/2)\sin^2(n_2\alpha_2/2)}{\sin^2(\alpha_1/2)\sin^2(\alpha_2/2)}$$

Whittle's Approximation

A very fast approximation of the likelihood of n realization of a Gaussian process with spectral density $f(k)$, is given by Whittle's approximation. According to this the negative log-likelihood is evaluated as

$$\frac{n_1 n_2}{4\pi^2} \sum_k \log f(k) + \frac{I(k)}{f(k)}$$

where the sum is over a collection of Fourier frequencies.

Whittle's Correlation

In a paper appeared in Biometrika 1954, Whittle advocates the use of the Matèrn correlation with $\nu = 1$ for processes in the plane. So this choice is known as the Whittle's correlation.

Consider the second order autoregressive scheme on a regular lattice

$$X(s_1, s_2) = \alpha(X(s_1 + 1, s_2) + X(s_1 - 1, s_2)$$

$$+X(s_1, s_2 + 1) + X(s_1, s_2 - 1)) + \varepsilon(s_1, s_2)$$

This can be written in the form

$$\left(\Delta^2_{s_1} + \Delta^2_{s_2} + \left(4 - \frac{1}{\alpha}\right)\right) X(s_1, s_2) = \varepsilon(s_1, s_2)$$

According to Whittle this is the simplest non-degenerate scheme on the plane.

A continuous analog is given by

$$\left(\frac{\partial^2}{\partial s_1^2} + \frac{\partial^2}{\partial s_2^2} - \kappa^2\right) X(s_1, s_2) = \varepsilon(s_1, s_2)$$

where ε denotes white noise. Using spectral analysis, Whittle calculates the correlation function of X and shows that it corresponds to the Matèrn with $\nu = 1$ and range $1/\kappa$.

Karhunen-Loève Representation

A Random process $X(s)$ can be represented as

$$X(s) = \sum_{j=1}^{\infty} \sqrt{\lambda_j}\psi_j(s)Z_j$$

where $E(Z_j Z_k) = \delta_{jk}$ and ψ_j is a basis of orthogonal functions such that

$$\int \psi_j(s)\overline{\psi_k(s)}ds = \delta_{jk}$$

and

$$\int C(s, s')\psi_j(s)ds = \lambda_j\psi_j(s')$$

So that λ_j is an eigenvalue of the covariance function and ψ_j the corresponding eigenfunction.

As a consequence of the previous representation we have that

$$C(s,s') = \sum_{j=1}^{\infty} \lambda_j \psi_j(s) \overline{\psi_j(s')}$$

Calculating the K-L expansion of a covariance function is a difficult task. As an illustration we have that for the exponential correlation function on the interval $[-L, L]$ and range $1/\phi$

$$\lambda_{j1} = \frac{2\phi}{w_{j1}^2 + \phi^2}, \quad \psi_{j1}(s) = \frac{\cos(w_{j1}s)}{\sqrt{L + \sin(2w_{j1}L)/(2w_{j1})}}$$

and

$$\lambda_{j2} = \frac{2\phi}{w_{j2}^2 + \phi^2}, \quad \psi_{j2}(s) = \frac{\sin(w_{j2}s)}{\sqrt{L - \sin(2w_{j2}L)/(2w_{j2})}}$$

where $w_{ji}, i = 1, 2$ solve $\tan(wL) = \phi/w$ and $\tan(wL) = -w/\phi$. Each one of these equations have an infinite number of solutions. They are obtained by intercepting the tangent $\tan(wL)$ with the functions ϕ/w and w/ϕ. The positive branch of the hyperbola gives $w_{\cdot 1}$. The straight line gives $w_{\cdot 2}$. Each intersection of the functions with a branch of the tangent gives a $w_{i\cdot}, i = 1, 2, \ldots$.

Empirical Orthogonal Functions

Suppose that the random function $X(s)$ is observed at locations $s_1, \ldots, s_m$. Let $\Gamma \in \mathbb{R}^{m \times m}$ be an empirical estimate of the covariance matrix for the vector $X(s_1), \ldots, X(s_m)$. Then we can write

$$\Gamma = P \Lambda P'$$

where Λ is a diagonal matrix of positive elements and P is an orthogonal matrix. Thus

$$\Gamma_{ij} = \sum_{k=1}^{m} \lambda_k P_{ik} P_{jk}$$

which is a discrete version of the K-L representation of C.

The columns of P are the **empirical orthogonal functions** of Γ.

We can approximate the random function as

$$X(s_i) \approx \sum_{j=1}^{M} \sqrt{\lambda_j} P_{ij} Z_j$$

A key element of this approximation is the availability of a good empirical estimate of the covariance matrix. In the absence of substantial prior information, this requires the availability of a good number of independent replicates of $X(s)$.

Eigenvalues and the Spectral Density

Consider a stationary correlation function ρ in $\mathbb{R}^n$. Then

$$\int \rho(s-t)e^{ik't}dt = e^{ik's}\int \rho(u)e^{-ik'u}du$$

So that $\lambda(k) = \int \rho(u)e^{-ik'u}du = f(k)$, the spectrum at k, is an eigenvalue and $e^{ik's}$ the corresponding eigenfunction of ρ.

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For a random process in $[-L, L]$ we have the approximation

$$\lambda_j \approx f(j\pi/(2L)) \quad \text{and} \quad \psi_j(t) \approx ce^{ij\pi t/(2L)}$$

where c is a normalizing constant.

Correlation Function on the Sphere

When working over large geographical domains it is natural to consider processes that are indexed by longitude and latitude. All valid isotropic correlation function on the sphere can be represented as

$$\rho(\theta) = \sum_{k=0}^{\infty} a_k P_k(\cos\theta), \quad \sum_{k=0}^{\infty} a_k = 1, \quad a_k \geq 0 \quad \theta \in [0, \pi]$$

where θ is the angular distance between two points in the sphere and P_k are the Legendre polynomials.

For example $P_0(u) = 1$, $P_1(u) = u$, $P_2(u) = (3u^2 - 1)/2$, $P_3(u) = u(5u^2 - 3)/2$.

Correlation Function on the Sphere

A practical way of obtaining a valid correlation function on the sphere is to take a correlation function in $\mathcal{D}_3$, say φ and define

$$\rho(\theta) = \varphi\left(2R\sin\left(\frac{\theta}{2}\right)\right)$$

where R is the radius of the sphere.

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Just substituting the angular distance for the Euclidean distance in a given correlation is not guaranteed to produce a valid correlation function on the sphere. For example, the Gaussian correlation function $\rho(\theta) = \exp\{-\phi\theta^2\}$ is NOT a valid correlation function on the sphere.

For computational efficiency it is very useful to consider covariance functions that are compactly supported. Furthermore, it is desirable that they are smooth function of the defining parameters.

A general strategy to obtain valid compactly supported correlations is to take the product

$$\psi_\alpha(\tau) = \rho_\nu\left(\frac{\tau}{\phi_\rho}\right)\varphi\left(\frac{\tau}{\phi}\right), \quad \alpha = (\nu, \phi_\rho, \phi)$$

where φ is a compactly supported correlation function.