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Nonparametric functionals of spectral distributions and their applications to time series analysis

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Abstract

There is a close analogy between empirical distributions of i.i.d. random variables and normalized spectral distributions of wide-sense stationary processes. Herein we make use of this analogy to develop nonparametric comparisons of two spectral distributions and nonparametric tests of stationarity versus change-point alternatives via spectral analysis of a time series.

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Keywords: Change point; Frequency domain; Linear process; Weak convergence

1. Introduction

Nonparametric testing in time series analysis has been one of Madan Puri's major areas of research; see Hall et al. (2003). Whereas work in this area are mainly concerned with the time domain, statistical analysis of electromyographic (EMG) signals has led us to nonparametric testing in the frequency domain. Section 2 reviews the background of EMG power spectra and statistical tests for spectral shifts associated with fatiguing muscle contractions. Ignoring the technical assumptions used for proving limit theorems, the frequency domain of time series analysis offers a richer arena for nonparametric methodology than the time domain since it only assumes wide-sense (i.e., mean and covariance) stationarity of the underlying time series and does not involve explicit ARMA modeling that is used in the nonparametric time-domain methods developed by Puri and others. Section 2 describes a variety of nonparametric functionals of spectral distributions and shows in particular how they can be used to test for spectral shifts. Closely related to the problem of nonparametric testing for differences in the spectral distributions associated with two stationary time series is that of nonparametric testing of stationarity versus change-point alternatives in spectral analysis of a time series, which is addressed in Section 3. Evaluation of boundary crossing probabilities of limiting Gaussian processes and fields to determine critical values of the test statistics is discussed in Section 4. Some concluding remarks are given in Section 5.

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2. Nonparametric functionals of spectral distributions and their applications

Let $X_1, X_2, \ldots, X_n$ be a zero-mean wide-sense stationary process. By the Wold decomposition,

$$X_t = \sum_{k=-\infty}^{\infty} a_k \varepsilon_{t-k}, \tag{2.1}$$

where ε_k are uncorrelated random variables with $E\varepsilon_i = 0$, $\mathrm{Var}(\varepsilon_i) = 1$ and a_k are nonrandom constants such that $\sum_{k=-\infty}^{\infty} a_k^2 < \infty$. Letting $\sigma(j) = \mathrm{Cov}(X_1, X_{1+j})$ be the autocovariance function and assuming that $\sum_{j=0}^{\infty} |\sigma(j)| < \infty$, the spectral density of X_t is given by

$$2\pi f(\omega) = \left| \sum_{k=-\infty}^{\infty} a_k \mathrm{e}^{\mathrm{i}k\omega} \right|^2 = \sigma(0) + 2 \sum_{j=1}^{\infty} \sigma(j) \cos j\omega, \quad -\pi \leqslant \omega \leqslant \pi. \tag{2.2}$$

Noting that $f(\omega) = f(-\omega)$, define the (normalized) spectral distribution function by

$$F(\theta) = \int_0^\theta f(\omega)\,\mathrm{d}\omega \Big/ \int_0^\pi f(\omega)\,\mathrm{d}\omega, \quad 0 \leqslant \theta \leqslant \pi. \tag{2.3}$$

In view of (2.2), $2\int_0^\pi f(\omega)\,\mathrm{d}\omega = \sigma(0)$. To estimate F, we replace $\sigma(j)$ by the sample covariance $\widehat{\sigma}_n(j) = n^{-1}\sum_{t=1}^{n-j} X_t X_{t+j}$ for $0 \leqslant j < n$ and $\widehat{\sigma}_n(j) = 0$ for $j \geqslant n$, which we then integrate from 0 to π to obtain the estimate

$$\widehat{F}_n(\theta) = \left\{ \theta \widehat{\sigma}_n(0) + 2 \sum_{j=1}^{n-1} \widehat{\sigma}_n(j)(\sin j\theta)/j \right\} \Big/ \{\pi \widehat{\sigma}_n(0)\}. \tag{2.4}$$

Note that $\widehat{\sigma}_n(j)/\widehat{\sigma}_n(0)$ is the sample autocorrelation at lag j.

The unnormalized spectral distribution $J(\theta) := \int_0^\theta f(\omega)\,\mathrm{d}\omega$ can be estimated by the numerator of the right-hand side of (2.4), which we denote by $\widehat{J}_n(\theta)$ and which is equal to $\int_0^\theta I_n(\omega)\,\mathrm{d}\omega$, where $I_n(\omega) = (2\pi n)^{-1} |\sum_{t=1}^n X_t \mathrm{e}^{\mathrm{i}t\omega}|^2$ is the periodogram that is used to estimate the integrand f of J. When the ε_n are i.i.d., (2.1) is called a *linear process*. Beginning with the seminal work of Grenander and Rosenblatt (1953, 1956, 1957), it has been shown that $\sqrt{n}(\widehat{J}_n - J)$ converges weakly to a Gaussian process W with mean 0 and covariance function

$$R(\theta, \theta') = (E\varepsilon_1^4 - 3) J(\theta) J(\theta') + 2\pi \int_0^{\theta \wedge \theta'} f^2(\omega)\,\mathrm{d}\omega \tag{2.5}$$

under a variety of regularity conditions; see Malevich (1964); Giraitis and Leipus (1990), Anderson (1993) and the references therein. Since $\widehat{F}_n(\theta) = \widehat{J}_n(\theta)/\widehat{J}_n(\pi)$, this weak convergence result for $\sqrt{n}(\widehat{J}_n - J)$ yields

$$\sqrt{n}(\widehat{F}_n - F) = \{\sqrt{n}(\widehat{J}_n - J) - \sqrt{n}(\widehat{J}_n(\pi) - J(\pi))F\}/\widehat{J}_n(\pi) \Longrightarrow (W - W(\pi)F)/J(\pi). \tag{2.6}$$

Moreover, since $F(\theta) = J(\theta)/J(\pi)$, it follows from (2.5) that

$$\begin{aligned} &E\{[W(\theta) - W(\pi)F(\theta)][W(\theta') - W(\pi)F(\theta')]\}/J^2(\pi) \\ &\quad = \{R(\theta, \theta') - F(\theta)R(\theta', \pi) - F(\theta')R(\theta, \pi) + F(\theta)F(\theta')R(\pi, \pi)\}/J^2(\pi). \end{aligned}$$

Noting that $J(\theta)J(\theta')$ in the four terms on the right-hand side of the above equality cancel one another, the covariance function of $Z := (W - W(\pi)F)/J(\pi)$ is

$$c(\theta, \theta') = 2\pi \left\{ \int_0^{\theta \wedge \theta'} \psi^2(\omega)\,\mathrm{d}\omega - F(\theta) \int_0^{\theta'} \psi^2(\omega)\,\mathrm{d}\omega - F(\theta') \int_0^{\theta} \psi^2(\omega)\,\mathrm{d}\omega + F(\theta)F(\theta') \int_0^{\pi} \psi^2(\omega)\,\mathrm{d}\omega \right\}, \tag{2.7}$$

where $\psi = f/J(\pi)$. In view of (2.7), we can represent the limiting process Z of $\sqrt{n}(\widehat{F}_n - F)$ as

$$Z(\theta) = \frac{\sqrt{2\pi}}{J(\pi)} \left\{ \int_0^\theta f(\omega)\,\mathrm{d}B(\omega) - F(\theta)\int_0^\pi f(\omega)\,\mathrm{d}B(\omega) \right\}, \quad 0 \leqslant \theta \leqslant \pi, \tag{2.8}$$

where B is Brownian motion. Note that $Z(0) = 0 = Z(\pi)$. In particular, for the "white noise" process $X_t = \varepsilon_t$, $f(\omega) = (2\pi)^{-1}$ and F is the uniform distribution function on $[0, \pi]$, so (2.8) reduces to $\sqrt{2/\pi}\,\{B(\theta) - (\theta/\pi)B(\pi)\}$, which is Brownian bridge on $[0, \pi]$. Therefore, the spectral distribution function $\widehat{F}_n$ of the white noise process has similar asymptotic behavior as that of the empirical distribution $\widehat{G}_n$ based on n i.i.d. random variables, suggesting that classical nonparametric methods based on $\widehat{G}_n$ can be readily extended to $\widehat{F}_n$. In particular, two-sample nonparametric tests of equality of two population distributions can be extended to compare the spectral distributions of two linear processes, as will be shown in Sections 2.2–2.4.

The (unnormalized) power spectrum $\widehat{J}_n$ can be retrieved from $\widehat{F}_n$ and the sample variance $\widehat{\sigma}_n(0)$. In many applications, such as those described at the end of Section 2.1, it is useful to test for spectral shifts (encoded in $\widehat{F}_n$) and for differences in total power (represented by $\widehat{\sigma}_n(0)$) when one power spectrum is compared against another. From (2.6), it follows that

$$(\sqrt{n}(\widehat{F}_n - F), \sqrt{n}[\widehat{\sigma}_n(0) - \sigma(0)]) \Longrightarrow (Z, \xi), \tag{2.9}$$

where ξ is a normal random variable with mean 0 and

$$\mathrm{Var}(\xi) = (E\varepsilon_1^4 - 3)\sigma^2(0) + 8\pi \int_0^\pi f^2(\omega)\,\mathrm{d}\omega \tag{2.10}$$

by (2.5), noting that $\widehat{\sigma}_n(0) = 2\widehat{J}_n(0)$. Moreover, $E\{Z(\theta)\xi\} = 0$ by (2.6), and therefore ξ is independent of $\{Z(\theta), 0 \leqslant \theta \leqslant \pi\}$ in view of joint normality. The asymptotic standard error of $\hat{\sigma}_n(0)$ is $n^{-1/2}$ multiplied by the square root of (2.10), which involves $\sigma(0)$ and $\int_0^\pi f^2(\omega)\,\mathrm{d}\omega$ that can be consistently estimated by $\widehat{\sigma}_n(0)$ and $\int_0^\pi \hat{\psi}_n^2(\omega)\,\mathrm{d}\omega$ (see (2.14) and the line following (2.15)). The term $E\varepsilon_1^4$ in (2.10) is difficult to estimate except in the white noise case $X_t = \varepsilon_t$ and in the Gaussian case (with $E\varepsilon_1^4 = 3$). Therefore, Grenander and Rosenblatt (1953) assume either white noise or Gaussian X_t in their application of (2.5) for the limiting Gaussian process to inference on the power spectrum J. Since $(E\varepsilon_1^4 - 3)J(\theta)J(\theta')$ can be expressed as $2\pi \int_0^\theta \int_0^{\theta'} f_4(\alpha, -\alpha, -\beta)\,\mathrm{d}\alpha\,\mathrm{d}\beta$, where f_4 is the fourth-order cumulant spectrum (cf. Politis et al., 1999, p. 169), one can approach the problem of estimating the term in (2.5) via consistent estimation of integral functionals of cumulant spectra, as in Taniguchi (1982) and Keenan (1987). Working with the normalized spectrum F instead of J circumvents the problem of estimating $E\varepsilon_1^4 - 3$, which no longer appears in (2.7).

For inference of $\sigma(0)$ based on $\widehat{\sigma}_n(0)$, we can avoid the estimation of $E\varepsilon_1^4$ by using subsampling to estimate the standard error of $\widehat{\sigma}_n(0)$. Specifically, let $v_{b,t}$ be the estimate $b^{-1}\sum_{i=t}^{t+b-1} X_i^2$ of $\sigma(0)$ based on the subsample $\{X_t, X_{t+1}, \ldots, X_{t+b-1}\}$, $1 \leqslant t \leqslant n - b + 1$. The sampling distribution of $\sqrt{n}[\widehat{\sigma}_n(0) - \sigma(0)]$ can be consistently estimated by the empirical distribution of $\{\sqrt{b}(v_{b,t} - \widehat{\sigma}_n(0)) : 1 \leqslant t \leqslant n - b\}$ as $n \to \infty$ and $b \to \infty$ such that $b/n \to 0$; see Politis et al. (1999, Section 3.2). Hence a consistent estimate of the standard deviation of $\sqrt{n}[\widehat{\sigma}_n(0) - \sigma(0)]$ is that of the subsample values.

2.1. *Statistical tests in EMG studies of muscle fatigue*

When an electrical impulse passes through a motor nerve and reaches a muscle, a muscle cell action potential is generated and the sum of action potentials of muscle fibers is known as the EMG signal. Sustained strong muscle contractions can cause muscle fatigue, and it has been well documented in the physiology literature that the spectral density of the EMG signal shifts towards lower frequencies during fatiguing contractions. Statistical tests based on the median frequency (Lindstrom et al., 1977), the centroid frequency (Schweitzer et al., 1979) and the high-to-low ratio (Gross et al., 1979) have been carried out in this literature by averaging the sample spectra either over subjects or over different time segments under similar physical conditions for fatigue (or rest), so that the traditional i.i.d. framework can be used without dealing with the dependence structure in (2.4).

In Sections 2.2–2.4 we consider direct comparison of the sample spectra of two linear processes by using (2.8), without generating independent replicates as in the above studies. The basic idea is similar to that of classical nonparametric tests of the equality of two population distributions, except that the asymptotic null variance of the test statistic is now more complicated but can still be estimated consistently. David et al. (1982) carried out a comparative study of the use of median versus mean (or centroid) frequency, and of the "high-to-low ratio" for the detection of muscle fatigue. Using the spectra averaged over data segments generated under similar experimental conditions, they found the centroid frequency to be most sensitive to fatigue. They also pointed out the importance and difficulty of an alternative statistical analysis based on a single time series rather than averaging over data segments to study the onset of fatigue.

In their study of diaphragmatic muscle fatigue during severe loaded breathing in adult sheep, Bazzy and Haddad (1984) found not only some shift in the centroid frequency during normal breathing but also more pronounced increase in total power. Haddad et al. (1986) subsequently undertook a more detailed analysis of the time course of total EMG power within three equal segments of a loaded breath, and the results suggest that during loaded breathing the recruitment pattern of diaphragmatic muscle fibers changes during the course of an inspiratory effort. Motivated by those applications, we extend the two-sample tests in Sections 2.2–2.4 to test for change-points in a sample spectrum in Section 3, which also addresses joint detection of shifts in F and changes in $\sigma(0)$.

2.2. The centroid frequency

Multiplying the right-hand side of (2.2) by $\theta/J(\pi)$ and then integrating from 0 to π gives an explicit formula for the centroid frequency $\mu=\int_0^\pi \theta\,\mathrm{d}F(\theta)$ in terms of the autocovariances $\sigma(j)$. Replacing $\sigma(j)$ by $\widehat{\sigma}_n(j)$ in the formula yields

$$\widehat{\mu}=\int_0^\pi \theta\,\mathrm{d}\widehat{F}_n(\theta)=\pi/2-4\sum_{1\leqslant j\leqslant n-1:\,j\text{ odd}}\widehat{\sigma}_n(j)/\{\pi j^2\widehat{\sigma}_n(0)\}, \tag{2.11}$$

which can be used to compute the sample mean frequency as an estimate of μ. In view of (2.8) and the continuous mapping theorem,

$$\sqrt{n}(\widehat{\mu}-\mu)=\sqrt{n}\int_0^\pi \theta\,\mathrm{d}(\widehat{F}_n-F)=-\int_0^\pi \sqrt{n}\{\widehat{F}_n(\theta)-F(\theta)\}\,\mathrm{d}\theta \tag{2.12}$$

converges weakly as $n\to\infty$ to

$$\begin{aligned}-\int_0^\pi Z(\theta)\,\mathrm{d}\theta&=\frac{\sqrt{2\pi}}{J(\pi)}\left\{\left(\int_0^\pi F(\theta)\,\mathrm{d}\theta\right)\int_0^\pi f(\omega)\,\mathrm{d}B(\omega)-\int_0^\pi(\pi-\omega)f(\omega)\,\mathrm{d}B(\omega)\right\}\\&=\{\sqrt{2\pi}/J(\pi)\}\int_0^\pi(\omega-\mu)f(\omega)\,\mathrm{d}B(\omega)\sim\mathrm{N}(0,v),\end{aligned} \tag{2.13}$$

where $v=2\pi\int_0^\pi(\omega-\mu)^2\{f(\omega)/J(\pi)\}^2\,\mathrm{d}\omega$. Whereas the periodogram $I_n(\omega)$ is an inconsistent estimate of f, a simple consistent estimate of f is obtained by "tapering" the $\widehat{\sigma}_n(j)$ that are used to estimate $\sigma(j)$ in (2.2). Specifically, we set $\widehat{\sigma}_n(j)=0$ not only for $j\geqslant n$ (with no observations available to estimate $\sigma_n(j)$) but also for $j>j_n$ with $j_n\to\infty$ but $j_n=\mathrm{o}(n)$, yielding a tapered estimate $\widehat{f_n}$ of f, or equivalently the tapered estimate

$$\widehat{\psi}_n(\omega)=\pi^{-1}\left\{1+2\sum_{j=1}^{j_n}(\widehat{\sigma}_n(j)/\widehat{\sigma}_n(0))\cos j\omega\right\} \tag{2.14}$$

of ψ; see Grenander and Rosenblatt (1957) and Brillinger (1981). Making use of (2.14), a consistent estimate of v is

$$\widehat{v}=2\pi\int_0^\pi(\omega-\mu)^2\widehat{\psi}_n^2(\omega)\,\mathrm{d}\omega, \tag{2.15}$$

in which the integral can be approximated by a Riemann sum with mesh size approaching 0 as $n\to\infty$. In view of the limiting normal distribution given by (2.13), approximate confidence intervals for μ can be constructed from the asymptotic pivot $(\widehat{\mu}-\mu)/\sqrt{\widehat{v}/n}$.

Note that more general linear functionals of the form $\int_0^\pi g(\theta)\,\mathrm{d}\widehat{F}_n(\theta)$ than the centroid frequency (2.11) can be treated similarly. Similar functionals $\int_0^\pi g(\theta)\,\mathrm{d}\widehat{J}_n(\theta)$ of the unnormalized spectrum $\widehat{J}_n$ have been considered by Brillinger

(1981, Section 7.6) and Keenan (1983), while related integral functionals of consistent estimators of f have been considered by Taniguchi et al. (1996) and Taniguchi and Kakizawa (2000, Chapter 6).

For the problem of testing for spectral shifts mentioned in the preceding section, let $\widehat{\mu}_1$ and $\widehat{\mu}_2$ be the sample estimates of the centroid frequencies μ_1 and μ_2 of two asymptotically independent linear processes and let $\widehat{v}_1$ and $\widehat{v}_2$ be the estimates of their respective limiting variances. Then the Studentized statistic

$$(\widehat{\mu}_1 - \widehat{\mu}_2)/\{\widehat{v}_1/n_1 + \widehat{v}_2/n_2\}^{1/2} \tag{2.16}$$

can be used to test the null hypothesis $\mu_1 = \mu_2$ (or the one-sided hypothesis $\mu_1 \leqslant \mu_2$), where n_1 and n_2 denote the respective sample sizes, as in t-tests based on sample means.

2.3. Median frequency, high-to-low ratio and linear combinations of spectral quantiles

For $0 < p < 1$, the pth quantile θ_p of the spectral distribution is the solution of the equation $F(\theta) = p$. Let $\widehat{\theta}_p$ be the corresponding quantile of the sample spectral distribution $\widehat{F}_n$. Since $\sqrt{n}(\widehat{F}_n - F) \Rightarrow Z$, application of the continuous mapping theorem shows that if $f(\theta_p) > 0$ then

$$\sqrt{n}(\widehat{\theta}_p - \theta_p) \Rightarrow Z(\theta_p)/\psi(\theta_p), \tag{2.17}$$

where $\psi = f/J(\pi)$ is the normalized spectral density. By (2.8),

$$\mathrm{Var}(Z(\theta_p)/\psi(\theta_p)) = \frac{2\pi}{\psi^2(\theta_p)}\left\{(1-p)^2\int_0^{\theta_p}\psi^2(\omega)\,\mathrm{d}\omega + p^2\int_{\theta_p}^{\pi}\psi^2(\omega)\,\mathrm{d}\omega\right\}. \tag{2.18}$$

Note the close analogy between (2.17) and (2.18) and the corresponding formulas for the pth quantile of the empirical distribution of a sample of n i.i.d. random variables, for which $Z(\theta)$ in (2.17) is replaced by a time-changed Brownian bridge. In fact, when f is the constant function, $Z(\theta)$ is Brownian bridge on $[0, \pi]$. As in the case of quantiles of empirical distributions, the limiting variance (2.18) of $\sqrt{n}(\widehat{\theta}_p - \theta_p)$ involves the normalized spectral density ψ, which we can estimate by (2.14) in order to apply the limiting normal distribution to hypothesis testing or confidence intervals. Moreover, the integrals in (2.17) can be approximated by Riemann sums, with the width of the subintervals partitioning $[0, \pi]$ approaching 0 as $n \to \infty$.

The case $p = \frac{1}{2}$ corresponds to the median frequency, for which the asymptotic variance in (2.18) reduces to $\pi\int_0^{\pi}\psi^2(\omega)\,\mathrm{d}\omega/(2\psi^2(\theta_p))$. Instead of the mean or median, consider a linear combination of spectral quantiles of the form

$$\ell_J = \int_0^{\pi}\theta J(F(\theta))\,\mathrm{d}F(\theta),$$

where J' is continuously differentiable on $[0, \pi]$. Replacing F in ℓ_J by $\widehat{F}_n$ yields the estimate $\widehat{\ell}_J = \int_0^{\pi}\theta J(\widehat{F}_n(\theta))\,\mathrm{d}\widehat{F}_n(\theta)$, for which

$$\begin{aligned}\sqrt{n}(\widehat{\ell}_J - \ell_J) &= \int_0^{\pi}\sqrt{n}\{J(\widehat{F}_n(\theta)) - J(F(\theta))\}\theta\,\mathrm{d}\widehat{F}_n(\theta) + \int_0^{\pi}\theta J(F(\theta))\,\mathrm{d}[\sqrt{n}(\widehat{F}_n - F)]\\ &\Rightarrow \int_0^{\pi}\theta J'(F(\theta))Z(\theta)\,\mathrm{d}F(\theta) + \int_0^{\pi}\theta J(F(\theta))\,\mathrm{d}Z(\theta) = -\int_0^{\pi}J(F(\theta))Z(\theta)\,\mathrm{d}\theta.\end{aligned} \tag{2.19}$$

To derive the last equality in (2.19), apply integration by parts to $\int_0^{\pi}\theta Z(\theta)\,\mathrm{d}J(F(\theta))$. Note that

$$\mathrm{Var}\left(\int_0^{\pi}J(F(\theta))Z(\theta)\,\mathrm{d}\theta\right) = \int_0^{\pi}\int_0^{\pi}J(F(\theta))J(F(\theta'))c(\theta,\theta')\,\mathrm{d}\theta\,\mathrm{d}\theta', \tag{2.20}$$

where $c(\theta, \theta')$ is given by (2.7). Using (2.14) to estimate ψ and $\widehat{F}_n$ to estimate F, and approximating the integral by a Riemann sum (with mesh size approaching 0 as $n \to \infty$), (2.20) and therefore also the standard error $\mathrm{se}(\widehat{\ell}_J)$ can be estimated consistently, yielding an approximately standard normal pivot $(\widehat{\ell}_J - \ell_J)/\widehat{\mathrm{se}}(\widehat{\ell}_J)$ that can be used to test hypotheses and construct confidence intervals for ℓ_J.

Section 2.1 has also considered the *high-to-low ratio*, which is $\{F(\omega_H) - F(\omega'_H)\}/\{F(\omega_L) - F(\omega'_L)\}$ and will be denoted by r, where $0 \leqslant \omega'_L < \omega_L < \omega'_H < \omega_H \leqslant \pi$ and (ω'_L, ω_L) represents a low-frequency band while (ω'_H, ω_H) a high-frequency band of the signal. This can be estimated by

$$\widehat{r} = \{\widehat{F}_n(\omega_H) - \widehat{F}_n(\omega'_H)\}/\{\widehat{F}_n(\omega_L) - \widehat{F}_n(\omega'_L)\}. \tag{2.21}$$

Making use of (2.8) and the delta method, it can be shown that $\sqrt{n}(\widehat{r} - r)$ has a limiting $\mathrm{N}(0, v)$ distribution, where

$$v = 2\pi \left\{ \int_{\omega'_H}^{\omega_H} \psi^2(\omega)\,\mathrm{d}\omega + r^2 \int_{\omega'_L}^{\omega_L} \psi^2(\omega)\,\mathrm{d}\omega \right\} \Big/ [F(\omega_L) - F(\omega'_L)]^2, \tag{2.22}$$

which can be estimated consistently by $\widehat{v}$ that replaces (ψ, F, r) by $(\widehat{\psi}_n, \widehat{F}_n, \widehat{r})$ and the integrals in (2.22) by Riemann sums. Therefore $(\widehat{r} - r)/\sqrt{\widehat{v}/n}$ has a limiting standard normal distribution.

2.4. Kolmogorov–Smirnov statistics

Anderson (1993) observed that $Z(\theta)/\sqrt{2\pi}$ can be expressed as a time-changed Brownian bridge as follows: Let $V(\theta) = \int_0^\theta \psi^2(\omega)\,\mathrm{d}\omega$ so that $\int_0^\theta \psi(\omega)\,\mathrm{d}B(\omega) \overset{\mathscr{L}}{=} B(V(\theta))$, and let $t = V(\theta)/V(\pi)$, $a(t) = F(\theta)$. Then $Z(\theta)/\sqrt{2\pi} \overset{\mathscr{L}}{=} \sqrt{V(\pi)}\{B(t) - a(t)B(1)\}$, since $B(ct) \overset{\mathscr{L}}{=} \sqrt{c}B(t)$. Therefore

$$\sqrt{n} \max_{0 \leqslant \theta \leqslant \pi} |\widehat{F}_n(\theta) - F(\theta)| \Rightarrow \max_{0 \leqslant \theta \leqslant \pi} |Z(\theta)| \overset{\mathscr{L}}{=} (2\pi V(\pi))^{1/2} \max_{0 \leqslant t \leqslant 1} |B(t) - a(t)B(1)|.$$

In practice $V(\pi)$ is unknown but can be consistently estimated by

$$\widehat{V} = \pi^{-1} \left\{ 1 + 2 \sum_{j=1}^{j_n} \widehat{\sigma}_n^2(j) \Big/ \widehat{\sigma}_n^2(0) \right\} \tag{2.23}$$

with $j_n \sim \sqrt{n}$; see Picard (1985, p. 845). Hence

$$(2\pi\widehat{V})^{-1/2} \max_{0 \leqslant \theta \leqslant \pi} \sqrt{n}|\widehat{F}_n(\theta) - F(\theta)| \Rightarrow \max_{0 \leqslant t \leqslant 1} |B(t) - a(t)B(1)|. \tag{2.24}$$

For the problem of comparing two spectral distributions F_1 and F_2, let $\widehat{F_1}$ and $\widehat{F_2}$ be the corresponding sample spectral distributions based on respective sample sizes n_1 and n_2. Then, as $n_1 \to \infty$ and $n_2 \to \infty$ such that n_1/n_2 converges to a positive limit, the preceding argument can be extended to yield that under the null hypothesis $F_1 = F_2$,

$$(2\pi\widehat{V})^{-1/2} \max_{0 \leqslant \theta \leqslant \pi} |\widehat{F}_1(\theta) - \widehat{F}_2(\theta)|/(n_1^{-1} + n_2^{-1})^{1/2} \Rightarrow \max_{0 \leqslant t \leqslant 1} |B(t) - a(t)B(1)|, \tag{2.25}$$

where $\widehat{V}$ is an estimate of the common $V(\pi) = \int_0^\pi \psi_i^2(\omega)\,\mathrm{d}\omega$ $(i = 1, 2)$, $t = V(\theta)/V(\pi)$ and $a(t) = F_1(\theta)(=F_2(\theta))$.

3. Testing stationarity versus change-point alternatives in a sample spectrum

In this section we modify the two-sample tests and their underlying weak convergence theory to develop spectral tests for change-points in a time series $X_1, \ldots, X_n$. The problem of testing the null hypothesis H_0 that $X_1, \ldots, X_n$ form a linear process with (unspecified) spectral density f versus the alternative hypothesis that there is a change-point m (unspecified) such that $(X_1, \ldots, X_m)$ and $(X_{m+1}, \ldots, X_n)$ have different spectral densities was studied by Picard (1985), who used an extension of the Kolmogorov–Smirnov test involving $\widehat{J}_m$ and the spectrum $\widehat{J}_{m,n-m}$ based on $X_{m+1}, \ldots, X_n$ (instead of $\widehat{F}_m$ and $\widehat{F}_{m,n-m}$).

To begin with, consider the alternative hypothesis that for some unspecified m, $(X_1, \ldots, X_m)$ and $(X_{m+1}, \ldots, X_n)$ have different variances.

3.1. Change-point tests based on the statistics in Sections 2.2 and 2.3

To begin with, consider the two-sample tests based on the Studentized difference (2.16) of mean frequencies. Letting $\{X_1, \ldots, X_m\}$ and $\{X_{m+1}, \ldots, X_n\}$ be the two samples, the means $\widehat{\mu}_m$ and $\widehat{\mu}_{m,n-m}$ of their spectra $\widehat{F}_m$ and $\widehat{F}_{m,n-m}$ can be used for the $\widehat{\mu}_1$ and $\widehat{\mu}_2$ in (2.16). Moreover, under H_0, $\widehat{v}_1$ and $\widehat{v}_2$ in (2.16) can be replaced by the estimate (2.15) of the common v of the entire time series. On the other hand, since m is unspecified, we can take the supremum of the Studentized difference over m between εn and $(1-\varepsilon)n$, with $0 < \varepsilon < \frac{1}{2}$, leading to the test statistic

$$M_n = \max_{\varepsilon n \leqslant m \leqslant (1-\varepsilon)m} \left\{ \frac{m(n-m)}{n\widehat{v}} \right\}^{1/2} |\widehat{\mu}_m - \widehat{\mu}_{m,n-m}| \tag{3.1}$$

that modifies the two-sample statistic (2.16) for testing H_0 versus change-point alternatives. As will be shown in Section 3.3,

$$M_n \text{ converges weakly to } \max_{\varepsilon \leqslant t \leqslant 1-\varepsilon} |B^0(t)|/\{t(1-t)\}^{1/2} \text{ under } H_0, \tag{3.2}$$

where $B^0(\cdot)$ denotes Brownian bridge on [0, 1], i.e., $B^0(t) = B(t) - tB(1)$. The restriction to $\varepsilon \leqslant m/n \leqslant 1-\varepsilon$ in (3.1) is closely related to the law of the iterated logarithm; it also reflects the need of enough data for consistent estimation of the means of the pre- and post-change spectra at the potential change-point m. More generally, we can replace $\{m(n-m)/n\}^{1/2} = \sqrt{n}\{m(n-m)/n^2\}^{1/2}$ in (3.1) by $\sqrt{n}\beta(m(n-m)/n^2) \geqslant 0$ such that

$$\int_0^{1/2} x^{-3/2} b(x) \exp(-b^2(x)/(2x))\, \mathrm{d}x < \infty, \quad \text{when } b(x) = 1/\beta(x), \tag{3.3}$$

leading to the test statistic $\widetilde{M}_n$ that rejects H_0 if $\widetilde{M}_n > c$, where

$$\widetilde{M}_n = \max_{1 \leqslant m \leqslant n} \sqrt{n/\widehat{v}}\beta(m(n-m)/n^2)|\widehat{\mu}_m - \widehat{\mu}_{m,n-m}|. \tag{3.4}$$

Then $\sup_{0<t<1} |B^0(t)|/b(t(1-t)) < \infty$ a.s. and

$$\widetilde{M}_n \text{ converges weakly to } \sup_{0<t<1} |B^0(t)|/b(t(1-t)) \text{ under } H_0, \tag{3.5}$$

as will be shown in Section 3.3.

The same idea can be used if the mean frequencies $\widehat{\mu}_m$ and $\widehat{\mu}_{n,n-m}$ are replaced by the median frequencies or more generally by the pth quantiles $\widehat{\theta}_m^{(p)}$ and $\widehat{\theta}_{m,n-m}^{(p)}$ of $\widehat{F}_m$ and $\widehat{F}_{m,n-m}$, or by linear combinations of quantiles associated with a weight function, or by the high-to-low ratios $\widehat{r}_m$ and $\widehat{r}_{m,n-m}$ associated with $\widehat{F}_m$ and $\widehat{F}_{m,n-m}$ via (2.18). In particular, the high-to-low ratios lead to the test statistic

$$\mathrm{HL}_n = \max_{1 \leqslant m \leqslant n} \sqrt{n/\widehat{v}}\beta(m(n-m)/n^2)|\widehat{r}_m - \widehat{r}_{m,n-m}|, \tag{3.6}$$

where $\beta \geqslant 0$ satisfies (3.3), $\widehat{v}$ is an estimate of the asymptotic variance (2.19) under H_0 based on the entire sample $X_1, \ldots, X_n$, and (3.5) still holds with $\widetilde{M}_n$ replaced by HL_n.

3.2. Change-point tests based on Kolmogorov–Smirnov-type statistics

Let $Y_n(t, \theta) = \sqrt{n}\{m(n-m)/n^2\}\{\widehat{F}_m(\theta) - \widehat{F}_{m,n-m}(\theta)\}$ for $t = m/n$ and define $Y_n(t, \theta)$ by linear interpolation for $(m-1)/n < t < m/n$, setting $Y_n(t, \theta) = 0$. It will be shown in Section 3.3 that

$$Y_n \text{ converges weakly in } C([0,1] \times [0,\pi]) \text{ to } Y, \tag{3.7}$$

in which Y is a zero-mean Gaussian random field with

$$\mathrm{Cov}(Y(t,\theta), Y(t',\theta')) = \{\min(t,t') - tt'\}c(\theta,\theta'), \tag{3.8}$$

where $c(\theta, \theta')$ is the covariance function (2.7) of Z. Making use of this, Section 3.3 also shows that

$$\begin{aligned} \mathrm{KS}_n &:= \max_{1\leqslant m\leqslant n} \sqrt{n/\widehat{V}}\beta(m(n-m)/n^2)\left\{\max_{0\leqslant\theta\leqslant\pi}|\widehat{F}_m(\theta)-\widehat{F}_{m,n-m}(\theta)|\right\} \\ &\Longrightarrow \sup_{0<t\leqslant 1/4, 0\leqslant s\leqslant 1} (2\pi V(\pi))^{1/2}|W(t,s)-a(s)W(t,1)|/b(t(1-t)) \end{aligned} \tag{3.9}$$

under H_0, where $\widehat{V}$ is the estimate of $V(\pi)$ given by (2.20), W is a tied-down Brownian sheet with $\mathrm{Cov}(W(t,s), W(t',s')) = \{\min(t,t') - tt'\}\min(s,s')$, and $a(s) = F(\theta)$ under the change of variables $s = V(\theta)/V(\pi)$. Therefore, the type I error probability of the test that rejects H_0 if $\mathrm{KS}_n > c$ can be approximated by

$$P\{|W(t,s)-a(s)W(t,1)| > cb(t(1-t)) \text{ for some } 0<t\leqslant 1 \text{ and } 0\leqslant s\leqslant 1\}, \tag{3.10}$$

whose computation is addressed in Section 4.

3.3. Derivations and joint detection of spectral shift and change in power

To prove (3.7), let $\{Z(t,\theta), 0\leqslant t\leqslant 1, 0\leqslant\theta\leqslant 2\pi\}$ be a zero-mean Gaussian process with $\mathrm{Cov}(Z(t,\theta), Z(t',\theta')) = \min(t,t')c(\theta,\theta')$, and let $Z_n(t,\theta) = m(\widehat{F}_m(\theta) - F(\theta))/\sqrt{n}$ for $t = m/n$, using linear interpolation for $(m-1)/n < t < m/n$. Recall that $F(\theta) = J(\theta)/J(\pi)$ and that $\widehat{F}_m(\theta) = \widehat{J}_m(\theta)/\widehat{J}_m(\pi)$, so the weak convergence of Z_n to Z follows, via the continuous mapping theorem as in (2.6), from that of $m(\widehat{J}_m - J)/\sqrt{n}$ established by Picard (1985) for normal ε_k and by Giraitis and Leipus (1990) under more general conditions. The weak convergence of Z_n to Z yields

$$\begin{aligned} &n^{-3/2}m(n-m)\{\widehat{F}_m(\theta) - \widehat{F}_{m,n-m}(\theta)\} \\ &= \left(1-\frac{m}{n}\right)\frac{m(\widehat{F}_m(\theta)-F(\theta))}{\sqrt{n}} - \frac{m}{n}\frac{(n-m)(\widehat{F}_{m,n-m}(\theta)-F(\theta))}{\sqrt{n}} \\ &\Rightarrow (1-t)Z(t,\theta) - t\{Z(1,\theta), Z(t,\theta)\} = Z(t,\theta) - tZ(1,\theta), \end{aligned}$$

which has the same covariance function as (3.8), completing proof of (3.7).

Applying (3.7) to the mean functional after integration by parts as in (2.12) yields (3.2). Since (3.3) is the Kolmogorov–Erdős–Feller integral test for b to belong to the upper class for Brownian motion, $\beta(t(1-t))B^0(t) = B^0(t)/b(t(1-t)) \to 0$ a.s. as $t(1-t) \to 0$ and (3.7) yields

$$\begin{aligned} &\sqrt{n/\widehat{v}}\,\{m(n-m)/n^2\}\left\{\int_0^\pi [\widehat{F}_m(\theta) - \widehat{F}_{m,n-m}(\theta)]\,\mathrm{d}\theta\right\}\Big/\, b(m(n-m)/n^2) \\ &\Longrightarrow \beta(t(1-t))v^{-1/2}\int_0^\pi Y(t,\theta)\,\mathrm{d}\theta \overset{\mathscr{L}}{=} \beta(t(1-t))B^0(t). \end{aligned} \tag{3.11}$$

To prove the equality (in distribution) above, note that

$$\begin{aligned} E\left\{\int_0^\pi\int_0^\pi Y(t,\theta)Y(t',\theta')\,\mathrm{d}\theta\,\mathrm{d}\theta'\right\} &= \{\min(t,t') - tt'\}\int_0^\pi\int_0^\pi c(\theta,\theta')\,\mathrm{d}\theta\,\mathrm{d}\theta' \\ &= \{\min(t,t') - tt'\}\mathrm{Var}\left(\int_0^\pi Z(\theta)\,\mathrm{d}\theta\right) = \{\min(t,t') - tt'\}v. \end{aligned}$$

From (3.11), (3.5) follows. A similar application of (3.7) can be used to prove (3.9), noting that under the transformation $s = V(\theta)/V(\pi)$ and $a(s) = F(\theta)$,

$$2\pi V(\pi)E[\{W(t,s) - a(s)W(t,1)\}\{W(t',s') - a(s')W(t',1)\}] = \mathrm{Cov}(Y(t,\theta), Y(t',\theta')),$$

in view of (3.8) and (2.7).

We next extend the preceding procedures and weak convergence arguments to the problem of joint detection of changes in $\sigma(0)$ and F. To begin with, consider the simpler problem of detecting change in $\sigma(0)$. In view of (2.9) (which gives an asymptotic normal distribution for $\widehat{\sigma}(0)$ analogous to (2.12) for $\widehat{\mu}$), we can use the test statistic

$$\Pi_n = \max_{1\leqslant m\leqslant n} \sqrt{n/\widehat{v}_b}\,\beta(m(n-m)/n^2)|\widehat{\sigma}_m(0) - \widehat{\sigma}_{m,n-m}(0)|, \tag{3.12}$$

where $\widehat{\sigma}_m(0)$ is estimated from $\{X_1, \ldots, X_m\}$, $\widehat{\sigma}_{m,n-m}(0)$ is based on $\{X_{m+1}, \ldots, X_n\}$ and $\widehat{v}_b$ is the sample variance of the subsample values $\{\sqrt{b}[b^{-1}\sum_{i=t}^{t+b-1} X_i^2 - \widehat{\sigma}(0)] : 1 \leqslant t \leqslant n-b\}$, which estimates (2.10) consistently if $b \to \infty$ but $b/n \to 0$ as $n \to \infty$. Under H_0, (3.5) still holds with $\widetilde{M}_n$ replaced by Π_n. Giraitis and Leipus (1990) have also derived (3.5) with $\widetilde{M}_n$ replaced by (3.12) in which $\beta(s) = s$ and $\widehat{v}_b$ is replaced by the right-hand side of (2.10).

For joint detection of changes in $\sigma(0)$ and F, we use the statistic Π_n to test for change in $\sigma(0)$ and a statistic T_n (which can be chosen from $\widetilde{M}_n$, HL_n and KS_n) to test for change in F. Under H_0, Π_n and T_n are independent; see the sentence following (2.10). Hence the type I error probability of the joint test that rejects H_0 if $T_n > c$ or $\Pi_n > c'$ is

$$P_{H_0}\{T_n > c \text{ or } \Pi_n > c'\} = P_{H_0}\{\Pi_n > c'\} + P_{H_0}\{T_n > c\}P_{H_0}\{\Pi_n \leqslant c'\}.$$

In particular, if we choose c' such that $P_{H_0}\{\Pi_n > c'\} \doteq \alpha/2$ using the Gaussian approximation, then for the joint test to have type I error probability α, we can use the Gaussian approximation to choose c such that $P_{H_0}\{T_n > c\} \doteq \alpha/(2-\alpha)$.

4. Evaluation of critical values via Gaussian process/field approximations

For exceedance probabilities of the Gaussian process in (2.24) or (2.25), Anderson (1993) observed that $B(t) - a(t)B(1) = B^0(t) - \widetilde{a}(t)X$, in which $\widetilde{a}(t) = a(t) - t$ and X is a standard normal random variable that is independent of the Brownian bridge $B^0(t)$. This enables one to compute $P\{\max_{0\leqslant t\leqslant 1} |B(t) - a(t)B(1)| > c\}$ by conditioning on X and using Durbin's (1973, Section 3.5) method for computing boundary crossing probabilities for Brownian bridge via numerical solution of a Volterra integral equation. It is, however, difficult to extend this method to multi-dimensional time for computing boundary crossing probabilities of the tied-down Brownian sheet in (3.9).

Asymptotic approximations to the boundary crossing probability $P\{|B^0(t)| > c\tilde{b}(t)$ for some $1 < t < 1\}$, with $\tilde{b}(t) = b(t(1-t))$ that is associated with the tail probability of $\widetilde{M}_n$ via (3.5), have been developed in the literature; see Siegmund (1986). For more general continuous Gaussian processes, Durbin (1985) developed an approximation to the density function of the first time that a Gaussian process crosses a boundary, which generalizes the following *tangent approximation* of Jennen and Lerche (1981) for the density function p_c of $T_c = \inf\{t \geqslant 0 : B(t) > b_c(t)\}$ for Brownian motion $B(\cdot)$:

$$p_c(t) \doteq t^{-3/2}\alpha_c(t)\varphi(b_c(t)/\sqrt{t}), \tag{4.1}$$

where $b_c > 0$ is continuously differentiable, φ is the standard normal density function and $\alpha_c(t) = b_c(t) - tb'_c(t)$. Note that in the case of a linear boundary $b_c(t) = \alpha + \beta t$ (with $\alpha > 0$ and $\beta > 0$), the well-known Bachelier–Lévy formula yields $p_c(t) = t^{-3/2}\alpha\varphi(b_c(t)/\sqrt{t})$, so the tangent approximation (4.1) simply replaces α by the intercept $\alpha_c(t)$ of the tangent line passing through $(t, b_c(t))$. For concave boundaries $b_c(t) = b(t)$ that become infinite as $t \to \infty$, one typically has $b'(t) = o(b(t)/t)$, so one can replace $\alpha_c(t)$ in (4.1) by $b(t)$, for which the right-hand side of (4.1) then reduces to the integrand in the integral test of (3.3). Instead of requiring the left-hand side of (4.1) to exist as a first exit density, Chan and Lai (2004) recently developed far-reaching generalizations of (4.1) by regarding its left-hand side as a "local" exit density at time t so that the probability that the process ever crosses the boundary within the time interval D is asymptotically equal to the integral of the right-hand side of (4.1) over D. In this way t can also be multi-dimensional, and the approximations to boundary crossing probabilities in Chan and Lai (2004) are in fact developed for Gaussian random fields, of which the Gaussian field $W(t,s) - a(s)W(t,1)$ in (3.9) is a special case.

5. Conclusion

Nonparametric functionals for the empirical distributions of i.i.d. random variables have their natural counterparts and associated weak convergence to Gaussian limits in the spectral distributions of linear processes. This was first noted by Grenander and Rosenblatt (1953) for the functionals $\max_{0\leqslant\theta\leqslant\pi} |\widehat{J}_n(\theta) - J(\theta)|$ and $\int_0^\pi (\widehat{J}_n(\theta) - J(\theta))^2\, d\theta$ that have weak convergence properties resembling those of the Kolmogorov–Smirnov and Cramér–von Mises statistics for empirical distributions. The resemblance can be even made much closer by using the normalized version $F = J/J(\pi)$ and its estimate $\widehat{F}_n$, as Anderson (1993) and Sections 2 and 3 have shown. In another direction, smoothing kernels and bandwidths for consistent spectral density estimation introduced by Bartlett (1948, 1950) were precursors of the theory of nonparametric density estimation developed later by Rosenblatt (1956) and Parzen (1962); see also Rosenblatt (1971). We have considered other functionals of $\widehat{F}_n$ besides the Kolmogorov–Smirnov functional, motivated by applications to the analysis of EMG signals for detecting the onset of muscle fatigue. These applications have also led us to the investigation of change-point problems associated with the sample spectra in Section 3, where we also consider joint detection of changes in F (indicating spectral shifts) and in $\sigma(0)$ (indicating increase or decrease in power).

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