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Enveloping Spectral Surfaces: Covariate Dependent Spectral Analysis of Categorical Time Series

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Abstract

Motivated by problems in Sleep Medicine and Circadian Biology, we present a method for the analysis of cross-sectional categorical time series collected from multiple subjects where the effect of static continuous-valued covariates is of interest. Toward this goal, we extend the spectral envelope methodology for the frequency domain analysis of a single categorical process to cross-sectional categorical processes that are possibly covariate dependent. The analysis introduces an enveloping spectral surface for describing the association between the frequency domain properties of qualitative time series and covariates. The resulting surface offers an intuitively interpretable measure of association between covariates and a qualitative time series by finding the maximum possible conditional power at a given frequency from scalings of the qualitative time series conditional on the covariates. The optimal scalings that maximize the power provide scientific insight by identifying the aspects of the qualitative series which have the most pronounced periodic features at a given frequency conditional on the value of the covariates. To facilitate the assessment of the dependence of the enveloping spectral surface on the covariates, we include a theory for analyzing the partial derivatives of the surface. Our approach is entirely nonparametric, and we present estimation and asymptotics in the setting of local polynomial smoothing.

Keywords

Circadian Biology; Optimal Scaling; Qualitative Time Series; Sleep Medicine; Spectral Analysis; Spectral Envelope

1 Introduction

Although the analysis of multiple time series has been studied extensively by statisticians and econometricians, the literature focuses primarily on series where the data are observational (e.g., stock prices). This has left a dearth of statistical methodology for the spectral analysis of multiple independent time series collected in experiments, especially in

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cases where the effect of non-dynamic covariates is of primary interest. The few methods that have been offered for the joint analysis of time series and non-dynamic covariates have been formulated exclusively for the analysis of quantitative time series and do not address the case where the time series are qualitative. The goal of this article is to offer a general theoretical framework and estimation procedure for analyzing the association between the second moment frequency properties of a qualitative time series and non-dynamic covariates observed from several independent subjects.

To motivate this statistical methodology, we consider a study in sleep medicine in which subjects are monitored during a night of sleep. For each subject, sleep was scored into epochs of rapid eye movement sleep (REM), non-rapid eye movement sleep (NREM), or wakefulness. Subjects completed a questionnaire that measures self-reported sleep quality, the Pittsburgh Sleep Quality Index (PSQI) (Buysse et al., 1989). Sleep quality, and more specifically the PSQI, has been shown to be associated with a multitude of aspects of functioning and general health. Understanding the dependency of the frequency domain properties of the qualitative time series of sleep staging on self-reported sleep quality will provide insight into electrophysiological correlates of sleep quality which can guide the development of clinical interventions.

The majority of current statistical methodologies for covariate dependent spectral analysis focus on analysis of power (ANOPOW) type problems where the covariate is a discrete grouping variable. An extensive discussion of some of the approaches to spectral regression and ANOPOW can be found in Shumway and Stoffer (2011, Chapter 7) while additional approaches are considered by Diggle and al Wasel (1997), Fokianos and Savvides (2008), and Stoffer et al. (2010). Krafty et al. (2011) introduced the mixed effects Cramér spectral representation as a general model for multiple time series which can account for the effect of both discrete valued grouping variables and continuous valued covariates.

All of the aforementioned methods are concerned exclusively with the spectral analysis of quantitative-valued time series. To the best of our knowledge, this article presents the first statistical methodology for analyzing the covariate dependent frequency domain properties of a qualitative time series. The most popular tool for the spectral analysis of categorical time series is the spectral envelope introduced in Stoffer, Tyler, and McDougall (1993). A review of the spectral envelope and its applications can be found in Stoffer, Tyler, and Wendt (2000). As with many approaches to the analysis of qualitative data, the spectral envelope begins by considering scalings which assign numerical values to each category of the qualitative random variables to produce univariate quantitative time series. The spectral envelope is then defined at each frequency as the as the maximum value of the normalized spectral density among all quantitative time series that can be obtained by scaling the qualitative time series. Subsequently, the power spectrum of the univariate quantitative time series obtained from any scaling divided by its variance is enveloped by the spectral envelope. We extend the ideas underlying the spectral envelope to introduce the enveloping spectral surface for describing the association between the frequency domain properties of a qualitative time series and covariates. The enveloping spectral surface offers an intuitively interpretable measure of association between covariates and a qualitative time series by finding the maximum possible normalized conditional power at a given frequency from

scalings of the qualitative time series conditional on the covariates. The optimal scalings which maximize the power provide scientific insight by identifying the aspects of the qualitative series which have the most pronounced periodic features at a given frequency conditional on the value of the covariates.

The enveloping spectral surface is defined for discrete, continuous, and mixed covariates. We focus primarily on the scenario where the covariates are continuous but offer a discussion about the enveloping spectral surface under other types of covariates. When faced with continuous covariates such that the distribution of power at a given frequency conditional on the covariates changes smoothly, the partial derivatives of the enveloping spectral surface with respect to the covariates provide a measure of how the maximal power at a given frequency obtained from scaling the qualitative time series depends on the covariates.

We propose a procedure for estimating the enveloping spectral surface and its derivatives which is based on local quadratic regression. Adhering to the traditional approach for the scaled analysis of qualitative valued random variables, we represent the qualitative time series as a vector valued time series through the use of indicator variables. Local quadratic smoothers are employed to obtain consistent estimates of the conditional variance matrix as well as the conditional spectral density matrix of the vector of indicator variables and its derivatives. A consistent estimate of the enveloping spectral surface is then obtained through the generalized singular value decomposition of the estimated multivariate spectral density with respect to the estimate of the variance matrix. The derivative estimate is used to obtain a consistent estimate of the partial derivatives of the enveloping spectral surface with respect to the covariate. Asymptotic distributions of the estimated enveloping spectral surface and its derivatives are derived and provided a means of performing large sample inference.

The rest of this article is organized as follows: Section 2 defines the theoretical setting and the enveloping spectral surface while Section 3 develops the estimation procedure for the enveloping spectral surface and its derivatives. Section 4 uses the spectral envelope to analyze the data from the sleep study. A discussion is presented in Section 5 while proofs are relegated to the Appendix.

2 Enveloping Spectral Surface

Consider a qualitative time series $\{X_{jt}; t = 0, \pm 1, \pm 2, \dots\}$ with finite state-space $C = \{c_1, c_2, \dots, c_{p+1}\}$ and a covariate vector $S_j = (S_{j1}, \dots, S_{jq})' \in S \subset \mathbb{R}^q$ from $j = 1, \dots, N$ independent subjects. We assume that $\{X_{jt}; t = 0, \pm 1, \pm 2, \dots\}$ is stationary conditional on S_j such that

$$\inf_{s \in \mathcal{S}, k=1, \dots, p+1} Pr \{X_{jt}=c_k | S_j=s\} > 0, \quad (2.1)$$

so that there are no absorbing states. The covariates S_j are assumed to be independent and identically distributed second order random variables with density function ϕ_s . Aside from making some smoothness assumptions about the conditional spectral distribution of X_{jt} given S_j to aid estimation, we will only assume a very general non-parametric model for X_{jt}

and S_j . Although this article is written for random covariates, the presented methodology and theory are applicable for deterministic covariates under appropriate technical assumptions.

In order to provide a quantifiable and rigorous measure of the spectral properties of the qualitative time series, consider the quantitative time series $X_{jt}(\beta)$ obtained from scaling X_{jt} with scalings $\beta = (\beta_1, \dots, \beta_{p+1})' \in \mathbb{R}^{p+1}$ such that $X_{jt}(\beta) = \beta_k$ when $X_{jt} = c_k$. Assuming the existence of the conditional spectral density of $X_{jt}(\beta)$ conditional on $S_j = s$ for all $\beta \in \mathbb{R}^{p+1}$, define

$$f_x(\omega, s; \beta) = \sum_{\tau=-\infty}^{\infty} \text{Cov}[X_{jt}(\beta), X_{jt+\tau}(\beta) | S_j = s] e^{-2\pi i \omega \tau}.$$

We want to choose a β that highlights some desirable characteristics of the distribution of X_{jt} conditional on $S_j = s$. As an extension of the spectral envelope for the analysis of a single qualitative time series, for every $\omega \in \mathbb{R}$ and $s \in S$, we define the enveloping spectral surface $\lambda(\omega, s)$ to be the maximal normalized conditional power among all possible scalings at frequency ω conditional on the covariate value $S_j = s$. Letting $V_x(s; \beta) = \text{Var}[X_{jt}(\beta) | S_j = s]$ be the conditional variance of the scaled time series and $\{1\} = \{a1; a \in \mathbb{R}\}$ be the subspace of $\mathbb{R}^{p+1}$ that is proportional to the vector of ones 1, we formally define the enveloping spectral surface as

$$\lambda(\omega, s) = \max_{\beta \in \mathbb{R}^{p+1} \setminus \{1\}} \frac{f_x(\omega, s; \beta)}{V_x(s; \beta)}. \quad (2.2)$$

In addition to the maximum value $\lambda(\omega, s)$, the scalings where this maximum is achieved can provide important information by locating the scalings of the qualitative time series for which cycles at a given frequency are most prominent conditional on the covariate vector. Note that scalings that assign the same value to each category are not considered since the variance of the resulting time series is zero and its normalized power spectral density is not well defined.

We name λ the enveloping spectral surface due to its form when S is a connected subspace of $\mathbb{R}^q$. In this setting, λ takes the form of the q -dimensional manifold which, when embedded in $\mathbb{R}^{q+1}$, envelopes the normalized conditional power spectrum at a given frequency and covariate vector for all scalings $\beta \in \mathbb{R}^{p+1} \setminus \{1\}$. Figure 2 displays the estimated enveloping spectral surface in the form of a 2-dimensional surface for the motivating sleep study where the covariate is the qualitative univariate covariate of the PSQI score. When S represents categorical grouping variables, such as sex or treatment type, λ has the form of multiple disconnected curves. The enveloping spectral surface offers just one possible extension of the spectral envelope for a single time series to our setting of multiple time series which are associated with non-dynamic covariates. A discussion about other formulations is given in Section 5.

2.1 A Computationally Convenient Formulation

A common tool for the analysis of qualitative random variables is to employ random vectors of indicator variables. Define the p -dimensional random vectors Y_{jt} which have a one in the k th element if $X_{jt} = c_k$ for $k = 1, \dots, p$ and zeros elsewhere. The existence of $f_x(\omega, s; \beta)$ for all $\omega \in \mathbb{R}$, $s \in S$, and $\beta \in \mathbb{R}^{p+1}$ assures the existence of the conditional spectral density of Y_{jt} . Define the conditional spectral density and variance of Y_{jt} as

$$f(\omega, s) = \sum_{\tau=-\infty}^{\infty} \text{Cov}(Y_{jt}, Y_{jt+\tau} | S_j = s) e^{-2\pi i \omega \tau}$$

$$V(s) = \text{Var}(Y_{jt} | S_j = s).$$

We will assume that $f(\omega, s)$ and $V(s)$ are non-singular for all $\omega \in \mathbb{R}$ and $s \in S$. It should be noted that the set of values of $\beta \in \mathbb{R}^{p+1} \setminus \{1\}$ which maximize $f_x(\omega, s; \beta)/V_x(s; \beta)$ is a multidimensional vector space. Representing X_{jt} through Y_{jt} is equivalent to setting the category c_{p+1} as a referent group and restricts the set of scalings where the enveloping spectral surface can be achieved to a lower dimensional space. This property is also present in the formulation of the spectral envelope and we direct readers to Stoffer, Tyler, and McDougall (1993) for a detailed discussion.

The spectral density matrix f completely describes the conditional second order spectral properties of X_{jt} given S_j . However, this p -dimensional multivariate positive definite Hermitian matrix indexed by $\mathbb{R} \times S$ is of such an unwieldy dimension that it is difficult to discern important information concerning the spectral relationship between X_{jt} and S_j from f alone. The enveloping spectral surface provides an easily interpretable low-dimensional representation of the information contained in f .

Since the spectral density is Hermitian, for every $\gamma \in \mathbb{R}^p$, $\gamma' f(\omega, s) \gamma = \gamma' f^{re}(\omega, s) \gamma$ where $f^{re}(\omega, s)$ is the real part of $f(\omega, s)$. This observation elucidates that the enveloping spectral surface and the scalings that achieve maximal normalized power can be computed through a generalized singular value decomposition over $\mathbb{R}^p$. The following lemma summarizes the connection between the formulation presented in this subsection to the enveloping spectral surface.

Lemma 1. For $\omega \in \mathbb{R}$ and $s \in S$, define the positive-definite $p \times p$ matrix

$$g(\omega, s) = V^{-1/2}(s) f(\omega, s) V^{-1/2}(s).$$

The enveloping spectral surface $\lambda(\omega, s)$ is the largest eigenvalue of $g^{re}(\omega, s)$. If $V^{1/2}(s)\gamma$ is an eigenvector of $g^{re}(\omega, s)$ associated with $\lambda(\omega, s)$, then

$$\begin{bmatrix} \gamma \\ 0 \end{bmatrix} \in \underset{\beta \in \mathbb{R}^{p+1} \setminus \{1\}}{\text{argmax}} \frac{f_x(\omega, s; \beta)}{V_x(s; \beta)}.$$

When the multiplicity of $\lambda(\omega, s)$ as an eigenvalue of $g^{re}(\omega, s)$ is one, there exists a unique $\gamma(\omega, s) \in \mathbb{R}^p$ such that $V^{1/2}(s)\gamma(\omega, s)$ is an eigenvector of $g^{re}(\omega, s)$ associated with (ω, s) such that $(\omega, s)'V(s)\gamma(\omega, s) = 1$ and the first non-zero entry of $\gamma(\omega, s)$ is positive.

2.2 Dependence of the Enveloping Spectral Surface on Covariate Values

An aspect of the enveloping spectral surface that can be of scientific interest are frequencies where the enveloping spectral surface changes based on covariate values. In our motivating sleep study, identifying the frequencies in the enveloping spectral surface that change with respect to sleep quality provides insight into the association between objectively measured sleep cycles and self-reported measures of sleep. If the enveloping spectral surface is the same regardless of covariate values, then there is no association between the maximal normalized power by scaling the qualitative time series and the covariates. An interpretable measure of the dynamics of the enveloping spectral surface with respect to the covariates depends on the form of the covariates. This article focuses on the case detailed in Assumptions 1 and 2 where the covariates are continuous random variables such that the spectrum $g^{re}(\omega, S)$ is smooth.

For a metric space D , let $\mathcal{C}^d(\mathcal{D})$ be the space of real valued functions over D such that all d th order partial derivatives exist and are continuous. We will make the following two smoothness assumptions.

Assumption 1. *The support of the density function ϕ_s is S and $\phi_s \in \mathcal{C}^2(\mathcal{S})$.*

Assumption 2. *Each element of the $p \times p$ spectral density matrix g^{re} is an element of the space $\mathcal{C}^4[\mathbb{R} \times S]$.*

Under Assumptions 1 and 2, the continuity of the eigenvalues of a matrix valued function imply that the enveloping spectral surface λ is continuous in both frequency and the covariates. In this setting, the first order partial derivatives of the enveloping spectral surface in the direction of the covariates provide an assessment of the dependence of the enveloping spectral surface on the covariates. Let $D\lambda(\omega, s)$ be the q -dimensional vector of partial derivatives of $\lambda(\omega, s)$ with respect to s which has k th element $D_k\lambda(\omega, s) = \lambda(\omega, s)/s_k$. For a frequency $\omega \in \mathbb{R}$, if $D\lambda(\omega, s) = \mathbf{0}$ for all $s \in S$, then there is no association between the the maximal amount of normalized power at frequency ω and the covariates. Lemma 2, which follows from Magnus and Neudecker (2007, Chapter 8, Theorem 7), provides a computationally useful form for $D_k\lambda$ in terms of the derivatives of the real part of the spectral density of the indicator variables.

Lemma 2. *Let $D_k g^{re}(\omega, s)$ be the $p \times p$ matrix with lm th element*

$D_k g_{\ell m}^{re}(\omega, s) = \partial g_{\ell m}^{re}(\omega, s) / \partial s_k$. Under Assumptions 1-2, if the multiplicity of $\lambda(\omega, s)$ as an eigenvalue of $g^{re}(\omega, s)$ is one, then

$$D_k \lambda(\omega, s) = \gamma(\omega, s)' V^{1/2}(s) D_k g^{re}(\omega, s) V^{1/2}(s) \gamma(\omega, s)$$

for $\omega \in \mathbb{R}$ and $s \in S$.

Lemma 2 provides a useful tool for developing an estimation procedure for the derivatives of the enveloping spectral surface directly from estimates of the eigenvectors and derivatives of g^{re} .

3 Estimation

3.1 Technical Assumptions and Notation

It is assumed that epochs of the qualitative time series of length T , $\{X_{jt}; t = 1, \dots, T\}$, are observed for $j = 1, \dots, N$ subjects. Asymptotic properties are established as both the number of time points and the number of subjects are large so that $T, N \rightarrow \infty$. Since the spectral density is Hermitian and periodic with period 1, we restrict our attention to $\omega \in [0, 1/2]$.

Estimation procedures based on multivariate local quadratic regression are proposed. Let K_q and K_{q+1} be spherically symmetric q and $q + 1$ -dimensional compactly supported density functions that possess eighth order marginal moments over S and $[0, 1/2] \times S$, respectively. For $k = q$ or $k = (q + 1)$, the bandwidth will be parameterized by assuming that there exists a positive definite $k \times k$ symmetric real matrix H^* and a scaling bandwidth $h > 0$ such that the bandwidth is parameterized as $H = hH^*$ and the corresponding weight functions are $|H|^{-1}K_k[H^{-1}s]$. Asymptotic properties will be established when $h \rightarrow 0$ as $N, T \rightarrow \infty$.

3.2 Estimation of V , g^{re} , and $D_k g^{\text{re}}$

Local quadratic estimation will be used to estimate V , g^{re} , and $D_k g^{\text{re}}$. A comprehensive review of local polynomial regression is given in Fan and Gijbels (1996). Although V , g^{re} , and its derivatives can be of scientific interest in their own right, this article is concerned with the estimation of these quantities exclusively for use in estimating and performing inference on the enveloping spectral surface and its derivatives.

To estimate V , let $\bar{Y}_j = T^{-1} \sum_{t=1}^T Y_{jt}$, $\tilde{V}_j = T^{-1} \sum_{t=1}^T (Y_{jt} - \bar{Y}_j) (Y_{jt} - \bar{Y}_j)'$, and $\tilde{V}_{j\ell m}$ be the ℓm th element of $\tilde{V}_j$. Additionally, let $\mathcal{Q}_k$ be the space of lower triangular real $k \times k$ matrices and $\text{vec}(Q)$ be a the k^2 -dimensional vector obtained by stacking the columns of the matrix $Q \in \mathcal{Q}_k$. The estimate $\hat{V}(s)$ of $V(s)$ is defined for every $s \in S$ as the $p \times p$ matrix with ℓm th element $\hat{V}_{\ell m}(s) = \hat{\alpha}_0$ such that

$$\begin{bmatrix} \hat{\alpha}_0 \\ \hat{\alpha} \\ \text{vec}(\hat{Q}) \end{bmatrix} = \underset{\alpha_0 \in \mathbb{R}, \alpha \in \mathbb{R}^q, Q \in \mathcal{Q}_{q+1}}{\text{argmin}} \sum_{j=1}^N \left\{ \tilde{V}_{j\ell m} - \alpha_0 - \alpha' (S_j - s) - (S_j - s)' Q (S_j - s) \right\}^2 \times K_q \left[H_v^{-1} (S_j - s) \right] / |H_v| \quad (3.3)$$

for a positive definite $q \times q$ symmetric matrix H_v . As $T \rightarrow \infty$, the estimates $\tilde{V}_j$ provide consistent estimates of $V(S_j)$ and we apply the local quadratic smoother to share information across independent subjects and to obtain estimates of $V(s)$ for all $s \in S$.

To estimate g^{re} and its derivatives, note that the conditional spectral density of $V^{-1/2}(S_j)Y_{jt}$ is $g(\omega, S_j)$. Define the normalized periodogram I_{jk} for $j = 1, \dots, N$ and $k = 1, \dots, [T/2]$ as

$$I_{jk} = \hat{V}^{-1/2}(S_j) \tilde{Y}_{jk} \tilde{Y}_{jk}^* \hat{V}^{-1/2}(S_j) \text{ where } \tilde{Y}_{jk} = T^{-1/2} \sum_{t=1}^T (Y_{jt} - \bar{Y}_j) e^{-2\pi i \omega_k t} \text{ is the finite}$$

Fourier transform of Y_{jk} at frequency $\omega_k = k/T$ and $\tilde{Y}_{jk}^*$ is the conjugate transpose of $\tilde{Y}_{jk}$. The components I_{jklm}^{re} provide asymptotically unbiased but inconsistent estimates of $g_{lm}^{re}(\omega_k, S_j)$ and we apply a local quadratic regression to these real components of the periodograms to obtain a consistent estimate of $g^{re}(\omega, s)$. For $\omega \in [0, 1/2]$ and $s \in S$, define the $p \times p$ matrices $\hat{g}^{re}(\omega, s)$ and $D_k \hat{g}^{re}(\omega, s)$ for $k = 1, \dots, q$ with respective lm th elements $\hat{g}_{lm}^{re}(\omega, s) = \hat{\alpha}_0$ and $D_k \hat{g}_{lm}^{re}(\omega, s) = \hat{\alpha}_{k+1}$ such that

$$\begin{bmatrix} \hat{\alpha}_0 \\ \hat{\alpha} \\ \text{vec}(\hat{Q}) \end{bmatrix} = \underset{\alpha_0 \in \mathbb{R}, \alpha \in \mathbb{R}^{q+1}, Q \in \mathcal{Q}_{q+1}}{\text{argmin}} \sum_{j=1}^N \sum_{k=0}^{\lfloor T/2 \rfloor} \left\{ I_{jklm}^{re} - \alpha_0 - \alpha' \begin{pmatrix} \omega_k - \omega \\ S_j - s \end{pmatrix} - \begin{pmatrix} \omega_k - \omega \\ S_j - s \end{pmatrix}' Q \begin{pmatrix} \omega_k - \omega \\ S_j - s \end{pmatrix} \right\}^2 K_{q+1} \left[H_g^{-1} \begin{pmatrix} \omega_k - \omega \\ S_j - s \end{pmatrix} \right] \quad (3.4)$$

$\hat{\alpha} = (\hat{\alpha}_1, \dots, \hat{\alpha}_{q+1})'$, and H_g is a symmetric positive definite $(q+1) \times (q+1)$ real matrix.

Theorem 1 provides the asymptotic consistency of $\hat{V}$, $\hat{g}^{re}$ and $D_k \hat{g}^{re}$ which will allow for consistent estimation of the enveloping spectral surface and its derivatives.

Theorem 1. Let $H_v = h_v H_v^*$ and $H_g = h_g H_g^*$ for positive definite symmetric matrices H_v^*, H_g^* and positive real numbers h_v, h_g . Under Assumptions 1 and 2, the first order optimal conditional mean squared error of $\hat{V}(s)$, $\hat{g}^{re}(\omega, s)$, and $D_k \hat{g}^{re}(\omega, s)$ for $\omega \in [0, 1/2]$ and $s \in S$ are achieved when $h_v \sim (NT)^{-1/(q+6)}$ and $h_g \sim (NT)^{-1/(q+7)}$ as $N, T \rightarrow \infty$. If $h_v \sim (NT)^{-1/(q+6)}$, $h_v \sim (NT)^{-1/(q+7)}$, and $N \sim T^{(q/6)-\varepsilon}$ for some $\varepsilon \in (0, q/6)$, then

$$\begin{aligned} \hat{V}(s) &= V(s) + O_p \left[(NT)^{-3/(q+6)} \right], \\ \hat{g}^{re}(\omega, s) &= g^{re}(\omega, s) + O_p \left[(NT)^{-3/(q+7)} \right], \\ D_k \hat{g}^{re}(\omega, s) &= D_k g^{re}(\omega, s) + O_p \left[(NT)^{-2/(q+7)} \right], \end{aligned}$$

conditional on $S_1, \dots, S_N$.

Large sample properties have been computed conditional on the covariates $S_1, \dots, S_N$ not only to aid interpretation but also because the marginal moments are not necessarily well defined. A discussion about the theoretical benefits in exploring the conditional properties of local polynomial estimates can be found in Ruppert and Wand (1994, Section 2).

The proposed element-wise local quadratic estimator is just one of several possible approaches to the estimation of V , g^{re} , and its derivatives. There are other approaches for the non-parametric estimation of a multivariate spectrum that could be readably extended to incorporate the covariate dimension. Extensions of the methods proposed by Dai and Guo (2004) and Rosen and Stoffer (2007) could provide consistent positive definite estimates of g which allow for different levels of smoothing for different components. We advocate the proposed local quadratic estimator for two reasons. First, it is computationally practical as compared to the computationally intensive Bayesian approach of Rosen and Stoffer (2007).

Second, it provides mathematically tractable estimates which allow for practical large sample inference as opposed to the Cholesky based estimation procedure of Dai and Guo (2004).

3.3 Estimation of $\lambda(\omega; s)$

Following the blueprint provided by Lemma 1 and Theorem 1 for the estimation of the enveloping spectral surface and optimal scalings, define $\hat{\lambda}(\omega, s)$ as the largest eigenvalue of $\hat{g}^e(\omega, s)$. Let $\hat{\gamma}(\omega, s) = \hat{V}^{-1/2}(s) \hat{\psi}(\omega, s)$ where $\hat{\psi}(\omega, s)$ is the eigenvector of $\hat{g}^e(\omega, s)$ associated with $\hat{\lambda}(\omega, s)$ such that $\hat{\gamma}(\omega, s)' \hat{V}(s) \hat{\gamma}(\omega, s) = 1$ and the first non-zero element of $\hat{\gamma}(\omega, s)$ is positive. Theorem 2 establishes the consistency and asymptotic distribution of $\hat{\lambda}(\omega, s)$ and the consistency of $\hat{\gamma}(\omega, s)$.

Theorem 2. *If Assumptions 1-2 hold, $h_v \sim (NT)^{-1/(q+6)}$, $h_g \sim (NT)^{-1/(q+7)}$ and $N \sim T^{(q/6)-\varepsilon}$ for some $\varepsilon \in (0, q/6)$ as $N, T \rightarrow \infty$, then for $\omega \in [0, 1/2]$ and $s \in S$*

$$\begin{aligned}\hat{\lambda}(\omega, s) &= \lambda(\omega, s) + O_p \left[(NT)^{-3/(q+7)} \right] \\ \hat{\gamma}(\omega, s) &= \gamma(\omega, s) + O_p \left[(NT)^{-3/(q+7)} \right]\end{aligned}$$

conditional on $S_1, \dots, S_N$. In addition, $\hat{\lambda}(\omega, s)$ is conditionally asymptotically normal with large sample variance

$$\text{Var} \left[\hat{\lambda}(\omega, s) | S_1, \dots, S_N \right] \approx \frac{\lambda^2(\omega, s) \rho}{NT |H_g| \phi_s(s)}$$

where

$$\begin{aligned}\rho &= (\mu_{14} - \mu_{12})^{-2} \left[\mu_{20} (\mu_{14} + \mu_{12}^2)^2 - 2(q+1) \mu_{12} \mu_{22} (\mu_{14} + q \mu_{12}^2) + (q+1) \mu_{12}^2 (\mu_{24} + q \mu_{22}^2) \right] \\ \text{for } \mu_{\ell m} &= \int_{\mathbf{u} \in \mathbb{R} \times \mathcal{S}} u_1^m K_{q+1}^\ell(\mathbf{u}) d\mathbf{u}.\end{aligned}$$

To aid in the identification of peaks in the enveloping spectral surface, we consider the first order Taylor series expansion where

$$\log \hat{\lambda}(\omega, s) \approx \log \lambda(\omega, s) + \frac{\hat{\lambda}(\omega, s) - \lambda(\omega, s)}{\lambda(\omega, s)}.$$

The large sample distribution of $\hat{\lambda}$ implies that $\log \hat{\lambda}$ is approximately normal with mean $\log \lambda(\omega, s)$ and variance $\rho/[NT|H_g|\phi_x(s)]$. If the qualitative time series were noise conditional on the covariates such that $\text{Cov}(Y_{jt}, Y_{jt+\tau} | S_j = s) = 0$ for all integers $\tau \neq 0$, then $g^{\text{re}}(\omega, s) = I$, $\lambda(\omega, s) = 1$, and $\log \lambda(\omega, s) = 0$ for all $\omega \neq 0$. Under this settings, we would expect $\hat{\lambda}(\omega, s)$ to be less than $z_{1-\alpha} \sqrt{\rho/[NT|H_g|\phi_x(s)]}$ approximately $(1 - \alpha) \times 100\%$ of the time where $z_{1-\alpha}$ is the $(1 - \alpha) \times 100$ percentile of the standard normal distribution. An empirical rule for

locating regions of the enveloping spectral surface of possible interest considers

combinations of ω and s such that $\hat{\lambda}(\omega, s) > \exp \left[z_{1-\alpha} \sqrt{\rho/NT |H_g| \phi_x(s)} \right]$. The density ϕ_s of the covariates may either be known from the study design or estimated from the observed data.

3.4 Estimation of $D\lambda(\omega; s)$

Lemma 2 can be used to obtain a consistent estimate of $D\lambda(\omega, s)$ from the estimates obtained in Sections 3.2 and 3.3. Define $\hat{D}\lambda(\omega, s)$ as the q -vector with k th element $\hat{D}_k\lambda(\omega, s)$ where

$$\hat{D}_k\lambda(\omega, s) = \hat{\gamma}(\omega, s)' \hat{V}^{1/2}(s) \hat{D}_k g^{re}(\omega, s) \hat{V}^{1/2}(s) \hat{\gamma}(\omega, s).$$

The consistency of $\hat{D}\lambda(\omega, s)$ and the large sample distribution of its elements are established in Theorem 3.

Theorem 3. *If Assumptions 1-2 hold, $h_v \sim (NT)^{-1/(q+6)}$, $h_g \sim (NT)^{-1/(q+7)}$ and $N \sim T^{(q/6)-\varepsilon}$ for some $\varepsilon \in (0, q/6)$ as $N, T \rightarrow \infty$, then for $\omega \in [0, 1/2]$ and $s \in S$*

$$\hat{D}\lambda(\omega, s) = D\lambda(\omega, s) + O_p \left[(NT)^{-2/(q+7)} \right]$$

conditional on $S_1, \dots, S_N$. In addition, $\hat{D}_k\lambda(\omega, s)$ is conditionally asymptotically normal with large sample variance

$$\text{Var} \left[\hat{D}_k\lambda(\omega, s) | S_1, \dots, S_N \right] \approx \frac{(e_k' H_g^{-2} e_k) \mu_{22}}{NT |H_g| \phi_s(s) \mu_{12}^2} \Gamma(\omega, S)$$

where e_k is the p -dimensional vector of zeros except for a one in k th element,

$$\mu_{\ell m} = \int_{\mathbf{u} \in \mathbb{R}^q \times \mathcal{S}} u_1^m K_{q+1}^\ell(\mathbf{u}) d\mathbf{u}, \text{ and } \Lambda(\omega, s) \text{ is uniquely determined by } g(\omega, s).$$

The explicit form for $\Lambda(\omega, s)$ is given in (A.2) in the Appendix. We note here that $\Lambda(\omega, s)$ depends on both $g^{re}(\omega, s)$ and $g^{im}(\omega, s)$. Subsequently, large sample confidence intervals for $D_k\lambda(\omega, s)$ require consistent estimates of both $g^{re}(\omega, s)$ and $g^{im}(\omega, s)$. An estimate for $g^{re}(\omega, s)$ has been obtained through $\hat{g}^{re}(\omega, s)$. The local quadratic smoother applied to the real part of the periodograms can be applied to the imaginary part to obtain an estimate of $g^{im}(\omega, s)$. The ensuing point-wise confidence intervals can be used to assess if, for a given frequency, the first derivatives in the direction of the covariates are different from zero and that the enveloping spectral surface at that frequency depends on the covariate vector.

4 Application: Spectral Analysis of Sleep Staging and Sleep Quality

4.1 Study Design

We consider data from the AgeWise study conducted at the University of Pittsburgh. The goal of the AgeWise study is to understand the connections between sleep and health, functioning, and well-being in older adults. Our current investigation considers data collected from $N=98$ adults between 60-89 years of age.

Each subject was monitored during a night of in-home sleep through ambulatory polysomnography. Polysomnography is a comprehensive recording of the electrophysiological changes that occur during sleep and includes the collection of electrocardiograph (ECG), electrocardiographic (EEG), electro-oculography (EOG), and electromyography (EMG) signals. The polysomnographic signals were used by a trained technician to score 20 second epochs into stages of rapid eye-movement sleep (REM), non-REM sleep, or wakefulness. Our analysis considers the six hours immediately following the onset of sleep. The resulting qualitative time series for each subject consists of sleep stage as one of the $p + 1 = 3$ categories of REM sleep, non-REM sleep, and wakefulness for each of the $T = 1080$ twenty second intervals during the first six hours after sleep onset. Sleep stages for two subjects are plotted in Figure 1.

In addition to polysomnography, each patient completed the PSQI questionnaire from which a PSQI score was computed. The PSQI, which was introduced by Buysse et al. (1989), is a common instrument for measuring self reported sleep quality. The PSQI questionnaire collects information about sleep quality and disturbance over a one month period. PSQI scores can take values between 0 and 21 with larger numbers representing poorer sleep quality. A score of 6 or larger has been shown to be clinically associated with poor sleep (Buysse et al., 1989; Cole et al., 2006). The observed PSQI scores in our sample of $N = 98$ subjects range from 1 to 16 with mean of 8.88 and standard deviation of 3.64.

The goal of our investigation is to determine the association between the frequency domain properties of sleep stages and the single, i.e. $q = 1$, quantitative variable of the PSQI score.

4.2 Analysis through the Enveloping Spectral Surface

We choose non-REM sleep as the referent group so that sleep stages for each subject are represented through indicator variables for wakefulness and for REM sleep. Local quadratic regression is implemented for the estimation of $\hat{\gamma}$ using the univariate Epanechnikov kernel and for the estimation of g^{te} using the spherical bivariate Epanechnikov kernel. The PSQI scores in our sample are approximately unimodal and symmetric; we estimate ϕ_s as the truncated normal distribution with support between 1 and 16, mean 8.88, and standard deviation 3.64.

The estimated enveloping spectral surface $\hat{\lambda}(\omega, \text{PSQI})$ displayed in Figure 2 indicates that power exists primarily within two frequency bands: a band of low frequencies between 0.17 and 0.23 cycles per hour, or between one cycle every 4 hours and 20 minutes and one cycle every 5 hours and 50 minutes, and a band of higher frequencies between 0.33 and 0.75 cycles per hour, or between one cycle every 1 hour and 20 minutes and one cycle every 3

hours. The estimated scalings $\hat{\gamma}$ where the power in the enveloping spectral surface is achieved are approximately equivalent to an indicator variable for wakefulness for frequencies in the low frequency band and approximately equivalent to an indicator variable for REM sleep for all frequencies in the higher frequency band. For example, the estimated optimal scaling at $\omega = 0.2$ cycles per hour and $\text{PSQI} = 2$ assigns the value 0.42 for awake, -0.09 for REM, and 0 for non-REM. The estimated optimal scaling at $\omega = 0.5$ cycles per hour and $\text{PSQI} = 6$ assigns the value 0.01 for awake, 0.37 for REM, and 0 for non-REM. To illustrate the scalings within these two bands, Figure 3 displays the estimated conditional spectra for wakefulness, or with the scaling that assigns a 1 to wakefulness and 0 to both REM and non-REM sleep, and for REM, or with the scaling that assigns a 1 to REM sleep and a 0 to both wakefulness and non-REM sleep.

To investigate if the power of the enveloping spectral surface within the frequency bands for wakefulness and for REM sleep changes with PSQI score, we compute the estimated partial derivative of the enveloping spectral surface with respect to PSQI score at frequencies $\omega = 0.2$ cycles per hour, or one cycle every 5 hours, and at $\omega = 0.5$, or one cycle every 2 hours. Figure 4 displays $\hat{D}\lambda(\omega = 0.2, \text{PSQI})$ and $\hat{D}\lambda(\omega = 0.5, \text{PSQI})$ along with estimated point-wise 95% confidence intervals. The estimated derivative at one cycle every 5 hours is negative for PSQI values less than 6 and not significantly different from zero for larger PSQI values. This indicates that the retaliative power in awakening every 5 hours decreases with an increase in PSQI for subjects with a PSQI less than 6 and is approximately the same for subjects with a PSQI greater than 6. Recall that the enveloping spectral surface is defined as the maximal normalized conditional power. From this result, we hypothesize that subjects awaken approximately every 5 hours regardless of their PSQI score but that subjects with a PSQI above 6 experience additional periods of wakefulness. Consequently, the normalized conditional power for wakefulness once every 5 hours is larger in subjects with smaller PSQI scores. The derivative of the enveloping spectral surface at the frequency of 1 cycle every 2 hours is not significantly different from zero and we conclude that the amount of conditional power of REM sleep at one cycle every 2 hours does not depend on PSQI score.

4.3 Results of the Analysis

The findings in our analysis may have additional applications in clinical sleep research. Individuals who complain of poor sleep quality do not consistently differ from individuals with good sleep quality in terms of traditional, visually-scored polysomnographic sleep variables such as the amount of wakefulness during sleep or the percentage of different sleep stages. Indeed, the initial validation of the PSQI showed only weak correlations between PSQI scores and such measures (Buysse et al., 1989). Our current findings suggest that objective correlates of poor subjective sleep quality may be more subtle than the gross quantitative measures typically examined. The temporal pattern of sleep and wakefulness is not adequately described with traditional polysomnographic variables, but is readily captured with the spectral surface methods described here. Thus, the key to understanding the objective correlates of subjective sleep quality may lie not in the amount of sleep and wakefulness, but in the temporal dynamics of sleep.

Other studies have also suggested that time series methods, including the rate of sleep-wake transitions (Punjabi et al., 2010) and survival analysis (Normal et al., 2006) may better correspond with subjectively restless sleep or the sleep disturbances caused by sleep apnea. These previous approaches examine the transitions between pre-specified states. In the context of our model, this is equivalent to the a priori selection of scalings. The flexibility of the enveloping spectral surface eliminates the need to pre-specify states of interests by locating optimal scalings. The results of our analysis suggest that the temporal aspect of the dynamics of sleep which is most correlated with self-reported sleep quality is the frequency of wakefulness throughout the night.

5 Discussion

In this paper, we extended the concept of scaling and the spectral envelope for analyzing qualitative-valued time series, which was introduced in Stoffer et al. (1993), to cross-sectional categorical processes that are possibly covariate dependent. The main goal was to determine the effect of continuous-valued covariates on the cyclic behavior of the series. Our approach was purely non-parametric and our estimation procedure was based on local polynomial smoothing.

The generality of our technique suggests approaches to other problems. For example, if the data $\{X_{jt}\}$ are quantitative-valued time series having a spectrum $f(\omega, s)$, then, in essence, the data are already scaled and one may proceed by estimating a spectral surface without having to perform the step in (2.2). In addition, if the data $\{X_{jt}\}$ are p -variate quantitative-valued series with spectral matrix $f(\omega, s)$, and one is willing to use a principal component approach, then one interest is in estimating the largest eigenvalue of the $p \times p$ spectral matrix, say $\lambda_1(\omega, s)$; of course, other eigenvalues may be of interest as well. For all intents and purposes, analysis based on the first spectral principal component is the problem solved here, although we focused primarily on the real part of the spectral matrix. In the multivariate case, the scaling vector $\beta(\omega, s)$ would now represent the corresponding loading vector at the particular frequency and value of the covariates.

An obvious extension to the problem presented here is the situation where the time series are grouped, so that we observe $\{X_{ijt}\}$ for $i = 1, \dots, I$ groups, $j = 1, \dots, N_i$ subjects in group i , and $t = 1, \dots, T$. If the goal is to consider the difference among groups, it may be possible to use the asymptotic normality of the group specific enveloping surfaces to perform pairwise group comparisons. It is difficult to say how one would include the information contained in the possibly different scalings produced by different groups. In this case, however, it may be possible to extend the work of Stoffer & Tyler (1998), who discussed scaling two categorical time series where the scales must be the same, to this case. The problem is related to spectral domain canonical correlation, but in this case, one is working with categorical time series.

Another problem of interest may be in reducing the dimension q by removing covariates. A possible solution would be to perform the procedure discussed here on all possible subsets and then choosing the best subset via some optimality criterion, although it is again difficult

to say how one would include the information contained in the different scalings produced by different sets of covariates.

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Appendix: Proofs of Theorems 1-3

All probabilistic statements in this Appendix are made conditional on $S_1, \dots, S_N$.

Proof of Theorem 1

Since $\tilde{V}_j = V(S_j) + O_p(T^{-1/2})$ uniformly for $S_j \in S$, Theorem 3 in Lu (1996) implies that the optimal mean square error is achieved when $h_v \sim (NT)^{-1/(q+6)}$ where $\hat{V}(s) = V(s) + O_p[(NT)^{-3/(q+6)} + O_p(T^{-1/2})]$. When $N \sim T^{(q/6)-\varepsilon}$, the error from approximating $V(S_j)$ with $\tilde{V}(j)$ is dominated in large samples by the error incurred from the local quadratic smoother.

To examine the properties of I_{jk} , note that (2.1) implies that all conditional moments of $V^{-1/2}(S_j)Y_{jt}$ exist and are bounded. Subsequently, the properties of multivariate periodograms established in Chapter 7 of Brillinger (1981) are applicable. Combining the properties of periodograms with the fact that $\hat{V}(s)$ is a consistent estimate of $V(s)$, for $l, m = 1, \dots, p$

$$I_{jklm}^{re} = g_{lm}^{re}(\omega_k, S_j) + g_{lm}^{re}(\omega_k, S_j) \varepsilon_{jklm} + O_p \left[(NT)^{-3/(q+6)} \right] \quad (\text{A.1})$$

where $\varepsilon_{j_1 k_1 l_1 m_1}$ and $\varepsilon_{j_2 k_2 l_2 m_2}$ are independent mean zero random variables with unit variance when $j_1 \neq j_2$ or $k_1 \neq k_2$. The theorem is completed by an application of Theorem 3 from Lu (1996) and noting that the error in approximating the distribution of the periodograms in (A.1), which is of the first order rate as the convergence of $\hat{V}$, is faster than the error incurred by applying the local quadratic smoother to the periodograms. This difference in convergence rates is a result of the local quadratic smoother for the periodograms being a $(q+1)$ -dimensional smoother while the local quadratic smoother for the estimation of V is a q -dimensional smoother.

Proof of Theorem 2

Theorems 3 and 4 from Lu (1996) establish the large sample variance and the asymptotic normality of $\hat{g}_{lm}^{re}(\omega, s)$. A direct extension of the proof of these theorems can be used in conjunction with Theorem 7.2.2 from Brillinger (1981), which shows that

$$\text{Cov} \left(I_{jkl_1 m_1}^{re}, I_{jkl_2 m_2}^{re} \right) = g_{l_1 l_2}^{re}(\omega_k, S_j) g_{m_2 m_1}^{re}(\omega_k, S_j) + g_{l_1 l_2}^{im}(\omega_k, S_j) g_{m_2 m_1}^{im}(\omega_k, S_j) + O \left[(NT)^{-3/(q+7)} \right] \quad (\text{A.2})$$

for $l_1, l_2, m_1, m_2 = 1, \dots, p$, to find that $\{\hat{g}_{\ell m}^{re}(\omega, s); \ell, m=1, \dots, p\}$ are jointly asymptotically normal with large sample covariance

$$Cov[\hat{g}_{l_1 m_2}^{re}(\omega, s), \hat{g}_{l_2 m_2}^{re}(\omega, s)] \approx \frac{\rho \left[g_{l_1 l_2}^{re}(\omega_k, s) g_{m_2 m_1}^{re}(\omega_k, s) + g_{l_1 l_2}^{im}(\omega_k, s) g_{m_2 m_1}^{im}(\omega_k, s) \right]}{NT|H_g|\phi_s(s)}.$$

Izenman (1975) discusses the Taylor series expansion of the largest eigenvalue and corresponding eigenvector of a symmetric matrix whose largest root is non-multiple. The application of this expansion to $\hat{g}^{re}(\omega, s)$ for establishing the consistency and asymptotic distribution of $\hat{\lambda}(\omega, s)$ and the consistency $\hat{\psi}(\omega, s)$ parallels its application for the spectral envelope. Details of this application can be found in the proof of Theorem 3.3 of Stoffer, Tyler, and McDougall (1993). The proof is then completed by using Slutsky's theorem to obtain the consistency of $\hat{\gamma}(\omega, s)$ from the consistency of $\hat{V}(s)$ and $\hat{\psi}(\omega, s)$.

Proof of Theorem 3

Consistency follows from Slutsky's theorem and the results of Theorems 1 and 2. A direct extension of the proofs of Theorems 3 and 4 from Lu (1996) using (A.2) shows that

$vec[D_k \hat{g}^{re}(\omega, s)]$ is asymptotically normal with large sample variance-covariance matrix

$$\frac{(e_k' H_g^{-2} e_k) \mu_{22}}{NT|H_g|\phi_s(s) \mu_{12}^2} (I+J) \left[g^{re}(\omega, s) \otimes g^{re}(\omega, s) + g^{im}(\omega, s) \otimes g^{im}(\omega, s) \right] / 2$$

where I is the $p^2 \times p^2$ identity matrix and $J = \sum_{\ell, m=1}^p (e_\ell e_m') \otimes (e_m e_\ell')$ is the $p^2 \times p^2$ permuted identity matrix. The asymptotic normality of $D_k \hat{\lambda}(\omega, s)$ follows after noting that

$$D_k \hat{\lambda}(\omega, s) = \left[\hat{\psi}'(\omega, s) \otimes \hat{\psi}'(\omega, s) \right] vec[D_k \hat{g}^{re}(\omega, s)] \left[\hat{\psi}'(\omega, s) \otimes \hat{\psi}'(\omega, s) \right]$$

where $\hat{\psi}(\omega, s) = \hat{V}^{1/2}(s) \hat{\gamma}(\omega, s)$ and that $\hat{\psi}(\omega, s)$ converges faster than $D_k \hat{g}_{\ell m}^{re}(\omega, s)$. Additionally,

$$Var[D_k \hat{\lambda}(\omega, s) | S_1, \dots, S_N] \approx \frac{(e_k' H_g^{-2} e_k) \mu_{22}}{NT|H_g|\phi_s(s) \mu_{12}^2} \Gamma(\omega, s)$$

where

$$\Gamma(\omega, s) = \left[\hat{\psi}'(\omega, s) \otimes \hat{\psi}'(\omega, s) \right] (I+J) \left[g^{re}(\omega, s) \otimes g^{re}(\omega, s) + g^{im}(\omega, s) \otimes g^{im}(\omega, s) \right] \left[\hat{\psi}(\omega, s) \otimes \hat{\psi}(\omega, s) \right] / 2 \quad (\text{A. } 2)$$

and $\psi(\omega, s)$ is the eigenvector of $g^{re}(\omega, s)$ associated with its largest eigenvalue.

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Figure 1.

Sleep stages from two subjects for the six hours following sleep onset. The plot on the left is from a subject with a PSQI score of 1 while the plot on the right is from a subject with a PSQI score of 15.

Figure 2.
The estimated enveloping spectral surface for sleep staging conditional on PSQI score.

Figure 3.
The estimated conditional power spectra of the time series of indicator variables for wakefulness and of the time series of indicator variables for REM sleep.

Figure 4.

The estimated partial derivatives and point-wise 95\% confidence intervals of the enveloping spectral surface for sleep staging with respect to the PSQI score for frequencies of one cycle every 5 hours and one cycle every 2 hours.