Nonparametric Covariance Estimation with Shrinkage Toward Stationary Models

Tayler Blake[*] Yoonkyung Lee[†]

Abstract
Estimation of an unstructured covariance matrix is difficult because of the challenges posed by parameter space dimensionality and the positive-definiteness constraint that estimates should satisfy. We consider a general nonparametric covariance estimation framework for longitudinal data using the Cholesky decomposition of a positive-definite matrix. The covariance matrix of time-ordered measurements is diagonalized by a lower triangular matrix with unconstrained entries that are statistically interpretable as parameters for a varying coefficient autoregressive model. Using this dual interpretation of the Cholesky decomposition and allowing for irregular sampling time points, we treat covariance estimation as bivariate smoothing and cast it in a regularization framework for desired forms of simplicity in covariance models. Viewing stationarity as a form of simplicity or parsimony in covariance, we model the varying coefficient function with components depending on time lag and its orthogonal direction separately and penalize the components that capture the nonstationarity in the fitted function. We demonstrate construction of a covariance estimator using the smoothing spline framework. Simulation studies establish the advantage of our approach over alternative estimators proposed in the longitudinal data setting. We analyze a longitudinal dataset to illustrate application of the methodology and compare our estimates to those resulting from alternative models.

Key Words: covariance estimation, nonparametric function estimation, longitudinal data, smoothing splines, reproducing kernel Hilbert space

1. Introduction

Estimation of a covariance matrix is fundamental to the analysis of multivariate data for mean inference, discrimination, and dimension reduction. The two primary challenges in fulfilling this prerequisite are due to the total number of parameters to be estimated in relation to the data dimension, and a structural constraint for covariance. As compared to mean estimation, the number of parameters grows quadratically in the dimension, and these parameters must satisfy the positive-definiteness constraint. It is well known that the widely used the sample covariance matrix, though positive-definite and unbiased for the population covariance matrix, is unstable in high dimensions [12]. In the applied literature, it is common practice to specify a parametric model for the covariance structure by incorporating primary factors for variation in the data or those elements suggested by a study design. These models are typically parsimonious and require modest computational effort for estimation. However, specifying the appropriate covariance model is challenging even for the experts, and model misspecification can lead to considerably biased estimates.

On the other hand, several regularized estimators of the sample covariance have been proposed to balance the two extremes. There are several elementwise regularization methods for estimating a covariance matrix; see, for example, [4, 5, 29, 23]. Methods for covariance estimation leveraging elementwise shrinkage are attractive, in part, because they typically present very low computational burden, but such estimators are not guaranteed to be positive-definite with finite sample sizes.

[*] The Ohio State University, Department of Statistics, Columbus, OH 43210

[†] The Ohio State University, Department of Statistics, Columbus, OH 43210

There has been a recent shift in covariance estimation toward regression-based approaches to eliminate the positive-definite constraint from estimation procedures altogether. Similar to this idea is the approach of modeling various matrix decompositions directly rather than the covariance matrix itself, including the spectral decomposition, the variance-correlation decomposition, and the Cholesky decomposition. The Cholesky decomposition in particular has recently received much attention because of its qualities that make it particularly attractive for its use in covariance estimation for data with naturally ordered measurements such as time series or longitudinal data. The entries of the lower triangular matrix and the diagonal matrix of the modified Cholesky decomposition have statistical interpretations as autoregressive coefficients, or the *generalized autoregressive parameters* and prediction variances, or *innovation variances* when regressing a measurement on its predecessors. The unconstrained reparameterization and its statistical interpretability makes it easy to cast covariance modeling into the generalized linear model framework while guaranteeing that the resulting estimates are positive-definite. See [21] for a general overview of modeling the Cholesky decomposition.

In this paper, we extend the regression model associated with the Cholesky decomposition of a covariance matrix to a functional varying coefficient model. Treating covariance estimation as bivariate smoothing, our framework naturally accommodates unbalanced longitudinal data and employs regularization as in the usual function estimation setting. The outline of the article is as follows. In Section 2, we review the role of the modified Cholesky decomposition in the unconstrained reparametrization of a covariance matrix. In Section 3, we present a functional varying coefficient model for the elements of the reparameterized covariance matrix and propose a reproducing kernel Hilbert space framework for estimation of the varying coefficient function. We demonstrate estimation of the innovation variances via smoothing splines in Section 4. Section 5 reviews a simulation study comparing the performance of our estimator to other covariance estimators proposed in the literature, and we apply our method to a dataset collected from a longitudinal study of cattle weights in Section 6.

2. The Cholesky Decomposition

For a positive-definite covariance matrix $\Sigma \in \mathbb{R}^{p \times p}$ for p variables, there exist a lower triangular matrix $T \in \mathbb{R}^{p \times p}$ with unit diagonal entries and a diagonal matrix $D \in \mathbb{R}^{p \times p}$ with positive entries such that

$$D = T \Sigma T'. \tag{1}$$

This representation (1) is commonly referred to as the modified Cholesky decomposition of Σ.

The lower triangular entries of T are unconstrained and can be interpreted as the coefficients of a particular regression model for ordered variables, and the diagonal of D can be interpreted as the prediction error variances associated with the same model. Let $Y = (y_1, \ldots, y_p)'$ denote a mean zero random vector with positive-definite covariance matrix Σ, and consider regressing y_t on its predecessors $y_1, \ldots, y_{t-1}$. Let $\hat{y}_t$ be the linear least-squares predictor of y_t based on previous measurements $y_{t-1}, \ldots, y_1$, and let $Var\left(\epsilon_t\right) = \sigma_t^2$ denote the variance of the corresponding prediction error, where $\epsilon_t = y_t - \hat{y}_t$. Regression theory gives us that there exist unique scalars ϕ_{tj} so that

$$y_t = \begin{cases} \epsilon_t, & t = 1 \\ \sum_{j=1}^{t-1} \phi_{tj} y_j + \epsilon_t, & t = 2, \ldots, p, \end{cases} \tag{2}$$

and the prediction errors ϵ_t are mean zero and independently distributed. If we negate the regression coefficients ϕ_{tj} and place them in the lower triangle of T so that the (t, j) entry of T is $-\phi_{tj}$, and let $D = \text{diag}\left(\sigma_1^2, \ldots, \sigma_p^2\right)$ and $\epsilon = (\epsilon_1, \ldots, \epsilon_p)'$, then the sequence of regression models in (2) can be written in matrix form as

$$\epsilon = TY. \tag{3}$$

Taking covariances on both sides of (3) gives the modified Cholesky decomposition (1). Thus, modeling a covariance matrix is equivalent to fitting a sequence of $p-1$ varying-coefficient and varying-order regression models. Since the ϕ_{tj} are regression coefficients, these and the $\log \sigma_t^2$, are unconstrained. The regression coefficients of the model in (2) are referred to as the *generalized autoregressive parameters* and *innovation variances* [19, 20]. The powerful implication of the regression framework of decomposition (1) is the accessibility of the entire portfolio of regression methods for the task of modeling covariance matrices. Moreover, the estimator $\hat{\Sigma}^{-1} = \hat{T}'\hat{D}^{-1}\hat{T}$ constructed from the unconstrained parameters, ϕ_{tj} and σ_t^2, is guaranteed to be positive-definite.

However, it is unclear how to apply Model (2) to irregular or incomplete data without prior imputation. In most longitudinal studies, the functional trajectories of the involved smooth random processes are not directly observable, and often, the observed data are sparse and irregularly spaced measurements of these trajectories. In the case that there is no fixed number of measurements and set of associated observation times for each subject, it is unclear how to define the discrete lag as in the usual formulation of autoregressive models. This makes treatment of individual subdiagonals of the Cholesky factor or the covariance matrix itself infeasible. To handle data collected in such a manner requires methods which are formulated in terms of continuous measurements. We address this concern by extending the framework supported by the unconstrained parameterization in (1) to naturally accommodate unbalanced longitudinal data. In the following section, we present a functional varying coefficient model for the elements of the Cholesky decomposition and propose regularization using a reproducing kernel Hilbert space framework.

3. A FUNCTIONAL VARYING-COEFFICIENT MODEL FOR THE MODIFIED CHOLESKY DECOMPOSITION

Given a sample of repeated measurements on N independent subjects, we model the observed data collected on an individual as a realization of a continuous-time stochastic process $Y(t)$ at discrete "time" points. In general, t doesn't need to be time, but for the ease of exposition, assume that measurements are indexed by time. Let $Y_i = (y(t_{i1}), \ldots, y(t_{i,p_i}))'$ denote measurements taken on the i^{th} subject at observation times $\mathcal{T}_i = \{t_{i1} < \cdots < t_{i,p_i}\}$, $i = 1, \ldots, N$. We assume that measurement times are drawn from $\mathcal{T} = [0, 1]$ without loss of generality.

We extend the linear model corresponding to the Cholesky decomposition (2) with the following functional varying-coefficient model:

$$y\left(t_{ij}\right) = \sum_{k<j} \tilde{\phi}\left(t_{ij}, t_{ik}\right) y\left(t_{ik}\right) + \epsilon\left(t_{ij}\right), \qquad \begin{array}{l} i = 1, \ldots, N \\ j = 2, \ldots, p_i, \end{array} \tag{4}$$

where the prediction errors $\epsilon\left(t\right)$ follow a mean-zero Gaussian process with variance function $\sigma^2\left(t\right)$. In the setting where sampling points are subject-specific and varying in length, the covariance function of the underlying process $Y(t)$, $\text{Cov}(Y(t), Y(s))$ becomes the natural target of interest.

As parsimonious parametric models, [20] and [17] considered low-order polynomials of the lag between observed time points for the generalized autoregressive coefficient function $\tilde{\phi}$ and polynomials of time for log innovation variances in the analysis of longitudinal data. Further, [27] proposed local polynomial smoothers to individually estimate the sub-diagonals of T for modeling $\tilde{\phi}$, imposing smoothnes along the direction of lag. Short-term dependence could be another form of parsimony for covariance models, and can be realized by truncating the varying coefficient at certain time lag, which leads to a banded matrix [11, 15].

The time lag or the sub-diagonal direction of T plays a prominent role in those parsimonious models for expressing the dependence structure. Rather than modelling the varying coefficient function $\tilde{\phi}$ directly, we reparameterize it explicitly in terms of lag and its orthogonal direction so that the fitted function can easily be used for suggesting parsimonious or structured models for the covariance function. Specifically, we take stationarity as a form of parsimony in covariance models, including those parameterizing the elements of T as a function of the lag between observations [14, 17, 19, 22]. To facilitate such model specification, we transform inputs from a pair of time points (t, s) for $t > s$ to the lag, $l = t - s \in [0, 1]$, and additive direction, $m = \frac{t+s}{2} \in [0, 1]$, and model ϕ in terms of the new arguments l and m:

$$\phi(l, m) \equiv \phi\left(t - s, \frac{1}{2}(s + t)\right) = \tilde{\phi}(t, s). \tag{5}$$

In other words, the composition of ϕ and the coordinate transformation yields $\tilde{\phi}$.

Model (4) corresponds to a stationary process when ϕ can be written as a function of lag l only and the innovation variances are constant in time t. For simplicity in the covariance model, we choose to regularize the autoregressive varying coefficient and the innovation variance function so that heavy penalization to both ϕ and σ^2 results in models which are close to stationary covariance matrices. To estimate $\phi(l, m)$ and $\sigma^2(t)$, we employ the smoothing spline framework [24].

In particular, we model ϕ in a structured function space that allows decomposition of ϕ into functional components of lag l and additive direction m, and using the components, we specify penalties that naturally yield the aforementioned models in the literature as null models. For such a structural representation of ϕ, we adopt the smoothing spline ANOVA models in [8] taken as a functional analogue of the classical analysis of variance (ANOVA) model. They exhibit the same interpretability as their classical counterparts, allowing multivariate functions to be decomposed into components similar in spirit to the main effects and interaction terms associated with the ANOVA model. This property makes them especially useful for verifying or eliciting parametric models [16].

3.1 Two-Way Functional ANOVA Models

To model the varying coefficient function ϕ on $[0, 1]^2$ using the smoothing spline ANOVA model framework, we first consider a univariate function space for lag l and additive direction m separately and take their tensor product. For example, the second-order Sobolev space $W_2[0, 1] = \{f : [0, 1] \to \mathbb{R} \,|f,\ f' \text{ absolutely continuous}, \int (f''(x))^2 dx < \infty\}$ can be taken as a model space for smooth univariate functions. When the curvature of f, $J(f) = \int_0^1 (f''(x))^2 dx$ is used as a roughness penalty functional for estimation of an unknown function from the space with data, the solution to the penalized least squares problem is known as a cubic smoothing spline. The function space $\mathcal{H} := W_2[0, 1]$ can be equipped with inner product such that $\mathcal{H}$ as a Hilbert space is a direct sum of two orthogonal subspaces $\mathcal{H}_0$ and $\mathcal{H}_1$, the null space $\mathcal{H}_0$ consists of constant or linear functions taken as null models, and the penalty functional $J(f)$ corresponds to the squared norm of the projection of f onto $\mathcal{H}_1$ denoted by $\|P_1 f\|^2$. Further, with an appropriate averaging operator (e.g. $A(f) = \int_0^1 f(x)dx$) and a basis $k_1(\cdot)$ for linear functions in $\mathcal{H}_0$ satisfying $A(k_1) = 0$

(e.g. $k_1(x) = x - 1/2$), the null space $\mathcal{H}_0$ can be decomposed as a direct sum of $\{1\}$ and $\{k_1(\cdot)\}$. Thus, $\mathcal{H} = \{1\} \oplus \{k_1(\cdot)\} \oplus \mathcal{H}_1$ and each function $f(x)$ in $\mathcal{H}$ admits a unique representation of $c_0 + c_1 k_1(x) + f_1(x)$ with $c_0, c_1 \in \mathbb{R}$ and $f_1 \in \mathcal{H}_1$. The functional decomposition is akin to the one-way ANOVA model. In the representation, $c_1 k_1(x) + f_1(x)$ is treated as a functional main effect of x, and $c_1 k_1(x)$ and $f_1(x)$ are called parametric and nonparametric main effects, respectively.

Taking two structured function spaces for l and m, $\mathcal{H}^{[l]} = \{1\} \oplus \{k_1(l)\} \oplus \mathcal{H}_1^{[l]}$ and $\mathcal{H}^{[m]} = \{1\} \oplus \{k_1(m)\} \oplus \mathcal{H}_1^{[m]}$ as building blocks, we can define the tensor product space $\mathcal{H}^{[l]} \otimes \mathcal{H}^{[m]}$ and use it as a model space for bivariate ϕ. Analogous to the two-way ANOVA model, the subspaces of $\mathcal{H}^{[l]} \otimes \mathcal{H}^{[m]}$ define a unique decomposition of ϕ into the overall mean, main effects of l and m, and interaction of l and m: $\phi(l, m) = \mu + \phi_1(l) + \phi_2(m) + \phi_{12}(l, m)$.

In addition, we can specify the null space as the subspace with desired simple models (e.g. low-order polynomials of lag only), and use the functional norm associated with each subspace to define a general "roughness" penalty functional $J(\phi)$ for bivariate smoothing, which results in two-way smoothing spline ANOVA models. This penalized function estimation framework is very flexible in the choice of a null space $\mathcal{H}_0$ and a penalty functional $J(\phi)$, allowing the user to adapt these choices to the context of data analysis and modeling.

Mathematically, smoothing spline ANOVA models are rooted in the theory of reproducing kernel Hilbert spaces [2, 24, 3]. Reproducing kernels are essential to the characterization of function spaces, their subspaces, and related geometric notion of norms and projections. For clear exposition of the model fitting procedure, we first review some basic properties of reproducing kernel Hilbert spaces.

3.2 Reproducing Kernel Hilbert Spaces

A Hilbert space $\mathcal{H}$ of functions on a set $\mathcal{X}$ with inner product $\langle \cdot, \cdot \rangle_{\mathcal{H}}$ is defined as a complete inner product linear space. For each $x \in \mathcal{X}$, let $[x]$ map $f \in \mathcal{H}$ to $f(x) \in \mathbb{R}$, which is known as the evaluation functional at x. A Hilbert space is called a reproducing kernel Hilbert space if the evaluation functional $[x] f = f(x)$ is continuous in $\mathcal{H}$ for all $x \in \mathcal{X}$. The Reisz Representation Theorem gives that there exists $K_x \in \mathcal{H}$, the representer of the evaluation functional $[x](\cdot)$, such that $\langle K_x, f \rangle_{\mathcal{H}} = f(x)$ for all $f \in \mathcal{H}$. See Theorem 2.2 in [8].

The symmetric, bivariate function $K(x_1, x_2) = K_{x_1}(x_2) = \langle K_{x_1}, K_{x_2} \rangle_{\mathcal{H}}$ is called the reproducing kernel (RK) of $\mathcal{H}$. The RK satisfies that for every $x \in \mathcal{X}$ and $f \in \mathcal{H}$, $K(x, \cdot) \in \mathcal{H}$, and $f(x) = \langle f, K(x, \cdot) \rangle_{\mathcal{H}}$. The second property is called the reproducing property of K. Every reproducing kernel uniquely determines the RKHS, and in turn, every RKHS has a unique reproducing kernel. See Theorem 2.3 in [8]. The representer of any bounded linear functional can be obtained from the reproducing kernel K. Further, if a reproducing kernel Hilbert space $\mathcal{H}$ is a direct sum of two orthogonal subspaces $\mathcal{H}_0$ and $\mathcal{H}_1$ with RKs K_0 and K_1, that is, $\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_1$, then the reproducing kernel for $\mathcal{H}$ is $K(x_1, x_2) = K_0(x_1, x_2) + K_1(x_1, x_2)$. See [2] for other RKHS properties.

3.3 Estimation of the Generalized Varying Coefficient Function via Bivariate Smoothing

For estimation of ϕ with data, we transform the observed time points to lags and additive directions. Given subject i and $j > k$, define $\boldsymbol{v}_{ijk} = \left(t_{ij} - t_{ik}, \frac{1}{2}\left(t_{ij} + t_{ik}\right)\right) = (l_{ijk}, m_{ijk}) \in \mathcal{V} = [0, 1]^2$ as the tuple corresponding to the transformed pair of j^{th} and k^{th}

observation times on the i^{th} subject. Let $V = \bigcup_{i,j,k} \{\boldsymbol{v}_{ijk}\} \equiv \left\{\boldsymbol{v}_1, \ldots, \boldsymbol{v}_{|V|}\right\}$ denote the set of unique within-subject pairs of observation times when pooled across N subjects.

We let the auto-regressive coefficient function ϕ belong to a reproducing kernel Hilbert space $\mathcal{H}$ with reproducing kernel K, which is structured as a tensor sum of the null space $\mathcal{H}_0$ and penalized space $\mathcal{H}_1$ with reproducing kernels K_0 and K_1, respectively. Let the penalty functional $J(\phi)$ measuring the complexity of ϕ, be $\|P_1\phi\|^2$, the squared norm of the projection of ϕ onto the subspace $\mathcal{H}_1$.

For example, consider $\mathcal{H} = \mathcal{H}^{[l]} \otimes \mathcal{H}^{[m]}$, where $\mathcal{H}^{[l]} = W_2[0,1] = \mathcal{H}_0^{[l]} \oplus \mathcal{H}_1^{[l]}$ with $\mathcal{H}_0^{[l]} = \{1\} \oplus \{k_1(l)\}$ and $\mathcal{H}^{[m]} = W_2[0,1] = \mathcal{H}_0^{[m]} \oplus \mathcal{H}_1^{[m]}$ with $\mathcal{H}_0^{[m]} = \{1\}$. This choice results in the null space $\mathcal{H}_0$ comprised of linear functions of lag only and amounts to penalizing the main effect of m, $\phi_2(m)$, and interaction of l and m, $\phi_{12}(l,m)$, altogether in addition to the curvature of the main effect of l. It has the effect of pulling estimated ϕ towards smooth functions of lag only treated as one form of parsimony in covariance modeling.

Under model (4), the negative log likelihood satisfies

$$-2\ell\left(\tilde{\phi}, \sigma^2 | Y_1, \ldots, Y_N\right) = \sum_{i=1}^{N}\sum_{j=1}^{p_i}\left[\log\sigma^2(t_{ij}) + \frac{1}{\sigma^2(t_{ij})}\left(y(t_{ij}) - \sum_{k<j}\tilde{\phi}(t_{ij}, t_{ik})y(t_{ik})\right)^2\right] \tag{6}$$

up to an additive constant.

Fixing the innovation variances $\sigma_{ij}^2 = \sigma^2(t_{ij})$, we take the estimator of ϕ to be the minimizer of the penalized negative log likelihood:

$$-2\ell\left(\phi | Y_1, \ldots, Y_N, \sigma^2\right) + \lambda J(\phi) = \sum_{i=1}^{N}\sum_{j=2}^{p_i}\frac{1}{\sigma_{ij}^2}\left(y(t_{ij}) - \sum_{k<j}\phi(\boldsymbol{v}_{ijk})\,y(t_{ik})\right)^2 + \lambda J(\phi), \tag{7}$$

where $\lambda > 0$ is a smoothing parameter, and denote it by ϕ_λ. The smoothing parameter λ controls the tradeoff between the goodness of fit measure ℓ and the penalty $\|P_1\phi\|^2$.

The following theorem establishes the form of the minimizer of the penalized negative log likelihood (7) and that the solution belongs to a finite-dimensional subspace despite the minimization being carried out over an infinite-dimensional space.

Theorem 1. *Let $\{\nu_1, \ldots, \nu_{\mathcal{N}_0}\}$ span $\mathcal{H}_0 = \{\phi \in \mathcal{H} : J(\phi) = 0\}$, the null space of $J(\phi) = ||P_1\phi||^2$. Then the minimizer ϕ_λ of* (7) *is of the form*

$$\phi_\lambda(\boldsymbol{v}) = \sum_{i=1}^{\mathcal{N}_0} d_i\nu_i(\boldsymbol{v}) + \sum_{j=1}^{|V|} c_j K_1(\boldsymbol{v}_j, \boldsymbol{v}), \tag{8}$$

where $K_1(\boldsymbol{v}_j, \boldsymbol{v})$ denotes the reproducing kernel for $\mathcal{H}_1$ evaluated at $\boldsymbol{v}_j$, the j^{th} element of V, viewed as a function of $\boldsymbol{v}$, $d_i \in \mathbb{R}$, and $c_j \in \mathbb{R}$.

This result is an example of the well-known representer theorem that holds for minimizers of regularized empirical risk functionals in a RKHS, and obtained by the standard argument with reproducing kernel properties. The proof is left to the Appendix. Using the representation of the minimizer, we discuss how to determine the coefficients d_i and c_j with data.

3.3.1 Model Fitting

Let $Y = \left(Y_1^{(-1)\prime}, Y_2^{(-1)\prime}, \ldots, Y_N^{(-1)\prime}\right)'$ denote the vector of length $n_Y = \sum_i p_i - N$, constructed by stacking the N observed response vectors, less their first element: $Y_i^{(-1)} = (y(t_{i2}), \ldots, y(t_{i,p_i}))'$. Define X_i to be the $(p_i - 1) \times |V|$ matrix containing the covariates for subject i necessary for regressing each measurement $y(t_{i2}), \ldots, y(t_{i,p_i})$ on its predecessors as in Model (4), and let $X = \begin{bmatrix} X_1' & X_2' & \ldots & X_N' \end{bmatrix}'$. Define K_V to be the $|V| \times |V|$ matrix with (i, j) entry given by $K_1\left(\boldsymbol{v}_i, \boldsymbol{v}_j\right)$, and let B denote the $|V| \times \mathcal{N}_0$ matrix with (i, j) element equal to $\nu_j\left(\boldsymbol{v}_i\right)$.

Assuming that σ_{ij}^2 are given for now, let D denote the $n_Y \times n_Y$ diagonal matrix of innovation variances σ_{ij}^2, and let $\tilde{Y} = D^{-1/2}Y$, $\tilde{B} = D^{-1/2}XB$, and $\tilde{K}_V = D^{-1/2}XK_V$. Using the representation of ϕ_λ in (8), and defining coefficient vectors $c = (c_1, \cdots, c_{|V|})'$ and $d = (d_1, \cdots, c_{\mathcal{N}_0})'$, the penalized negative log likelihood in (7) is given by

$$-2\ell\left(c, d|\tilde{Y}, \tilde{B}, \tilde{K}_V\right) + \lambda J\left(\phi\right) = \left[\tilde{Y} - \tilde{B}d - \tilde{K}_V c\right]'\left[\tilde{Y} - \tilde{B}d - \tilde{K}_V c\right] + \lambda c' K_V c. \quad (9)$$

For fixed smoothing parameter, setting partial derivatives with respect to d and c equal to zero, the solution ϕ_λ is obtained by finding c and d which satisfy:

$$\begin{bmatrix} \tilde{B}'\tilde{B} & \tilde{B}'\tilde{K}_V \\ \tilde{K}_V'\tilde{B} & \tilde{K}_V'\tilde{K}_V + \lambda K_V \end{bmatrix} \begin{bmatrix} d \\ c \end{bmatrix} = \begin{bmatrix} \tilde{B}'\tilde{Y} \\ \tilde{K}_V'\tilde{Y} \end{bmatrix}. \quad (10)$$

When $\tilde{K}_V$ is full column rank, the solution can be obtained through the Cholesky decomposition of the symmetric matrix on the left side of the equality in (10). Writing

$$\begin{bmatrix} \tilde{B}'\tilde{B} & \tilde{B}'\tilde{K}_V \\ \tilde{K}_V'\tilde{B} & \tilde{K}_V'\tilde{K}_V + \lambda K_V \end{bmatrix} = CC',$$

the solution is given by $\begin{bmatrix} \hat{d}' & \hat{c}' \end{bmatrix}' = C^{-1}(C')^{-1} \begin{bmatrix} \tilde{B} & \tilde{K}_V \end{bmatrix}' \tilde{Y}$. Singularity of $\tilde{K}_V$ demands special computational consideration to solve (10). For detailed examination, we refer the reader to [9].

The appropriate choice of smoothing parameter λ is crucial for effectively recovering the true ϕ. In practice, a number of data-driven methods are available for model selection such as the Akaike or Bayesian information criterion [6] or cross validation-based procedures [24, 9] including the leave-one-subject-out cross validation (losoCV) criterion for repeated measures data [28].

4. Estimation of the Innovation Variance Function via Smoothing Splines for Exponential Families

Given an estimate of ϕ, we can estimate the innovation variance function $\sigma^2(t)$, using the corresponding innovation errors as the new data residuals as the working innovation errors. If the true innovations $\epsilon(t_{ij})$ were given, then the joint likelihood in (6) would reduce to

$$-2\ell\left(\sigma^2|Y_1, \ldots, Y_N, \phi\right) = \sum_{i=1}^{N}\sum_{j=1}^{p_i}\left(\log\sigma^2(t_{ij}) + \frac{\epsilon^2(t_{ij})}{\sigma^2(t_{ij})}\right) \quad (11)$$

for estimation of $\sigma^2(t)$. The fact that $\epsilon^2(t_{ij})$ is a scaled chi-square random variable and the form of the likelihood above motivate a variance model for $\sigma^2(t)$ with the $\epsilon^2(t_{ij})$ serving as the response using Gamma distributions. When a Gamma distribution with shape parameter

α and scale parameter β is reparametrized with mean parameter $\mu = \alpha\beta$ in place of β, a negative log likelihood of μ based on a single observation z from the distribution is shown to be proportional to $\alpha\left(\log\mu + \frac{z}{\mu}\right)$ with $1/\alpha$ treated as a fixed dispersion parameter. Recognizing the connection between the Gamma likelihood and (11), we cast estimation of the innovation variance function in a generalized linear model framework with Gamma errors and fixed shape parameter. Further, to remove the constraint that $\mu > 0$, we transform μ to $\eta = \log\mu$ and reparametrize the Gamma likelihood as $\alpha\left[\eta + z\exp(-\eta)\right]$.

Defining $\eta(t) = \log\sigma^2(t)$ and assuming a smooth log innovation variance function, we use the smoothing spline method for regression relating squared innovations, $\epsilon^2(t_{ij})$, as Gamma responses to time points t_{ij}. Generalized smoothing spline models that relate the canonical parameter of an exponential family to a set of covariates have been studied extensively. See [25], [26], and [8].

As with the estimation of the functional varying coefficient, estimation is carried out by minimizing the penalized negative log likelihood with the working innovation errors. Given ϕ^*, an estimate of ϕ, define the working innovation errors, $\hat{\epsilon}(t_{ij}) = y(t_{ij}) - \sum\limits_{k<j}\phi^*\left(\boldsymbol{v}_{ijk}\right)y(t_{ik})$, and the corresponding squared innovations, $z_{ij} \equiv z(t_{ij}) = \hat{\epsilon}^2(t_{ij})$. Let $Z_i = (z(t_{i1}), \ldots, z(t_{i,p_i}))'$ denote the vector of squared innovations for the i^{th} observed trajectory. With $Z_1, \ldots, Z_N$, the negative log likelihood of $\eta(t)$ becomes

$$-2\ell\left(\eta|Z_1, \ldots, Z_N\right) = \sum_{i=1}^{N}\sum_{j=1}^{p_i}\left(\eta(t_{ij}) + z_{ij}e^{-\eta(t_{ij})}\right). \qquad (12)$$

Similar to the estimation of ϕ, we consider a function space $\mathcal{H}$ for $\eta(t)$ on $[0,1]$ with an orthogonal decomposition of $\mathcal{H}_0 \oplus \mathcal{H}_1$ and define a roughness penalty $J(\eta)$ that can be written as the squared norm of the projection of η to $\mathcal{H}_1$. For instance, take $\mathcal{H} = W_2[0,1]$ with $J(\eta) = \int_0^1(\eta'(t))^2dt$ which corresponds to $\mathcal{H}_0 = \{1\}$. Combining the likelihood with the penalty, we define our estimator of $\eta(t)$ to be the minimizer of the penalized negative log likelihood:

$$-2\ell\left(\eta|Z_1, \ldots, Z_N\right) + \lambda J\left(\eta\right) = \sum_{i=1}^{N}\sum_{j=1}^{p_i}\left(\eta(t_{ij}) + z_{ij}e^{-\eta(t_{ij})}\right) + \lambda J\left(\eta\right). \qquad (13)$$

The first term in (13) serves as a measure of the goodness of fit of η to the data, and only depends on η through the evaluation of η at observed time points. Thus, the argument justifying the form of the minimizer in (8) applies to η. Let $\mathcal{T}_{obs} = \bigcup_{i,j}\{t_{ij}\}$ denote the unique values of the observations times pooled across subjects. The minimizer of the penalized likelihood (13) has the form

$$\eta_\lambda\left(t\right) = \sum_{i=1}^{\mathcal{N}_0} d_i\nu_i\left(t\right) + \sum_{j=1}^{|\mathcal{T}_{obs}|} c_jK_1\left(t_j, t\right), \qquad (14)$$

where $\{\nu_i\}$ form a basis for the null space $\mathcal{H}_0$ and $K_1\left(t_j, t\right)$ is the reproducing kernel for $\mathcal{H}_1$ evalutated at t_j, the j^{th} element of $\mathcal{T}_{obs}$, viewed as a function of t.

To jointly estimate the autoregressive coefficient function and the innovation variance function, we adopt an iterative approach in the spirit of [11], [10], and [20]. A procedure for minimizing

$$-2\ell\left(\phi, \eta|Y_1, \ldots, Y_N\right) + \lambda_\phi J_\phi\left(\phi\right) + \lambda_\eta J_\eta\left(\eta\right)$$

starts with initializing $\eta(t_{ij}) = 0$ or $\sigma_{ij}^2 = \exp(\eta(t_{ij})) = 1$ for $i = 1, \ldots, N, j = 1, \ldots, p_i$. For fixed η, we find ϕ^* minimizing the penalized negative log likelihood

$$-2\ell\left(\phi | Y_1, \ldots, Y_N, \eta\right) + \lambda_\phi J_\phi\left(\phi\right).$$

Given ϕ^*, we update our estimate of η by taking η^* that minimizes the penalized negative log likelihood with the working squared residuals

$$-2\ell\left(\eta | Z_1, \ldots, Z_N, \phi^*\right) + \lambda_\eta J_\eta\left(\eta\right).$$

This process of iteratively updating ϕ^* and η^* is repeated until convergence.

5. Simulation Studies

In this section we compare our bivariate spline estimator to other methods of covariance estimation through simulation studies with generative models. Our primary comparisons are that with the polynomial estimator for ϕ and σ^2 proposed by [17]. Their approach, which is also based on the Cholesky decomposition, permits unbalanced data without requiring missing data imputation. However, the polynomial estimator assumes that $\tilde{\phi}(t, s)$ can be parameterized as a (univariate) polynomial in $l = t - s$ only. Thus, discrepancies in the performance of the estimators may be indicative of situations in which our parameterization (5) is advantageous. We also consider the performance of the oracle estimator under each of the generating models, the sample covariance matrix and two of its regularized variants: the tapered sample covariance matrix [5] and the soft thresholding estimator [23], neither of which rely on a natural ordering among the variables.

We consider the following five covariance structures for the data generating distribution. The covariance functions as two-dimensional surfaces corresponding to each generating model are shown left to right in Figure 1. The first row displays the surface coinciding with the appropriate discrete covariance matrix on a 10×10 grid, and the second row displays the surfaces of the corresponding Cholesky factors (the lower triangle of $-T$). The precise model definitions are in Table 1. When Σ is not directly specified in the table, the covariance matrices in Figure 1 are obtained by either evaluating the covariance function $\sigma(t, s)$ at 10 equally spaced points, $\{t_1, \cdots, t_{10}\}$, from $[0, 1]$ or numerically constructing $\Sigma = T^{-1} D T'^{-1}$ after forming T and D from the specified $\tilde{\phi}(t, s)$ and $\sigma^2(t)$.

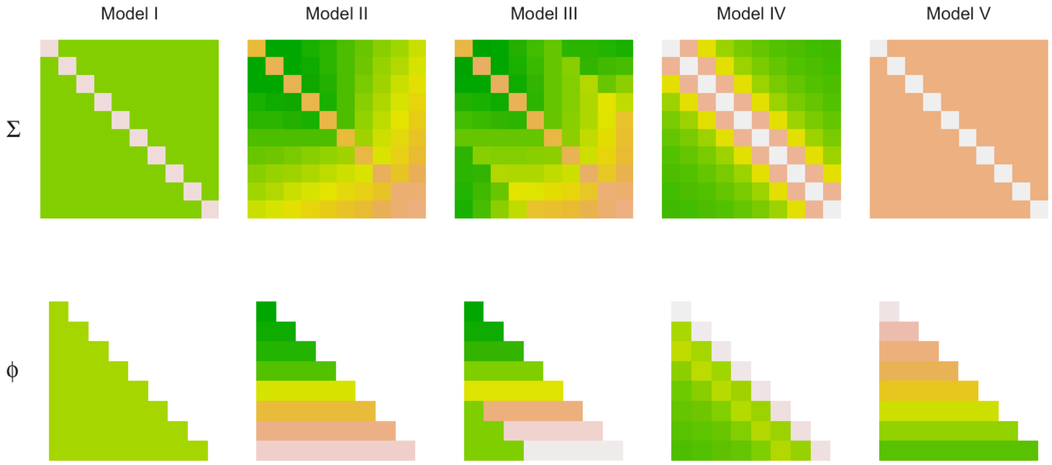


Figure 1: *Heatmaps of the true covariance matrices corresponding to Model I - Model V and ϕ defining the corresponding Cholesky factor T. The smallest elements of each matrix correspond to dark green pixels; the light pink (white) pixels correspond to the large (largest) elements of the matrix.*

Model	Σ or $\sigma(t,s)$	$\tilde{\phi}(t,s)$ for $t > s$	$\sigma^2(t)$
I: Independence	I	0	1
II: Linear Coefficient	$*$	$t - 0.5$	0.1^2
III: Banded Linear	$*$	$\begin{cases} t - 0.5 & \text{if } t - s \leq 0.5 \\ 0 & \text{if } t - s > 0.5 \end{cases}$	0.1^2
IV: Rational Quadratic	$\left(1 + \frac{(t-s)^2}{2k^2}\right)^{-1}$ with $k = 0.6$	$*$	$*$
V: Compound Symmetry	$(1-\rho)\,\mathrm{I} + \rho\mathrm{J}$ with $\rho = 0.7$	$\tilde{\phi}(t_j, t_k) = \frac{\rho}{1+(j-2)\rho}$ for $j > k$	$\sigma^2(t_j) = 1 - \frac{(j-1)\rho^2}{1+(j-2)\rho}$

Table 1: *Covariance models for data generation. The true covariance function $\sigma(t,s)$, varying coefficient function $\tilde{\phi}(t,s)$, and innovation variance function $\sigma^2(t)$ are defined with the domain $\mathcal{T} = [0,1]$. The asterisks indicate that the entries are determined numerically when discretized.*

Under each of the five covariance models, we generate data from a mean zero p-variate Normal distribution with covariance matrix $\Sigma = T^{-1}DT'^{-1}$ and construct an estimate of Σ for each combination of $p = 10, 20, 30$ and sample size $N = 50, 100$. Since construction of the sample covariance matrix S and regularized variants S^{ω} (tapered) and S^{λ} (soft-thresholded) requires an equal number of observations on each subject taken at a common set of observation times, simulations were conducted using complete data, with observation times $t = 1, \ldots, p$ mapped to the unit interval. The smoothing spline estimator $\hat{\Sigma}_{SS}$ was constructed by using a tensor product cubic smoothing spline for ϕ and univariate cubic smoothing spline for $\sigma^2\left(t\right)$.

[19] parsimoniously models the generalized autoregressive coefficients and the innovation variances as low-order polynomials in l and t respectively. [17] extend their work, proposing an estimator $\hat{\Sigma}_{poly}$ which allows for subject-specific observation times. They model $\phi_{ijk} = z'_{ijk}\gamma$ and $\log \sigma^2_{ij} = h'_{ij}\xi$, where the elements of z_{ijk} and h_{ijk} contain poly-

nomials bases of order q and d evaluated at l_{ijk} and t_{ij}, respectively. The regression parameters γ and ξ are estimated via maximum likelihood, and the optimal pair of polynomial orders (q, d) is selected using Bayesian criterion information (BIC).

To assess performance of an estimator $\hat{\Sigma}$, we consider the entropy loss

$$\Delta\left(\Sigma, \hat{\Sigma}\right) = tr\left(\Sigma^{-1}\hat{\Sigma}\right) - \log|\Sigma^{-1}\hat{\Sigma}| - p,$$

which can be derived from the Wishart likelihood [1]. Given Σ, we prefer the estimator with the smallest risk, $R\left(\Sigma, \hat{\Sigma}\right) = E_{\Sigma}\left[\Delta\left(\Sigma, \hat{\Sigma}\right)\right]$. To evaluate the risk via Monte Carlo approximation, we generate 100 replicates of $\hat{\Sigma}$ and calculate the corresponding average loss.

Figure 2 provides a visual summary of the qualitative differences between the estimates resulting from each of the six methods of estimation for the five covariance structures used for simulation. The first row in the grid shows the surface plot of each of the true covariance structures, and each row thereafter corresponds to the five covariance estimates for the given estimation method; oracle estimators for each covariance model were constructed assuming that the structure of the underlying generating model is known. For example, the oracle estimator of the covariance matrix corresponding to mutual independence with constant variance is a diagonal matrix with the diagonal elements given by $\hat{\sigma}^2$, which is an estimate of the variance based on all of the data, $\{y_{ij}\}$. For each simulation setting, the risk of the oracle estimator serves as a lower bound on the risk for the given covariance structure.

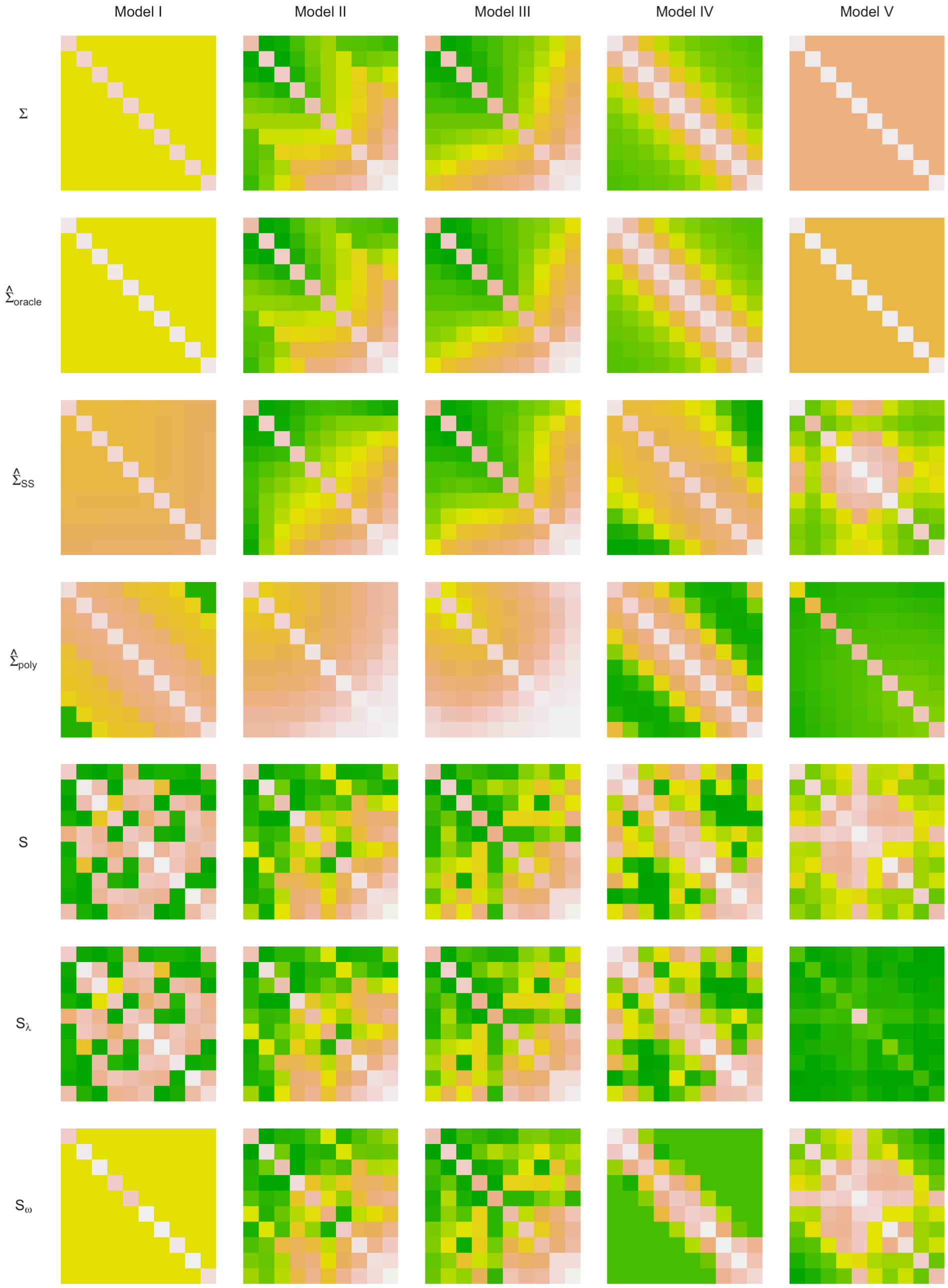


Figure 2: *Covariance Model I - Model V used for simulation and corresponding estimates with various methods. True covariance structures are shown in the first row followed by their estimates from the oracle estimator, smoothing spline ANOVA estimator, parametric polynomial estimator, the sample covariance matrix, the tapered sample covariance matrix, and the soft thresholding estimator.*

A summary of the estimated entropy risk for the covariance estimators is presented in Table 2. Smoothing parameters for $\hat{\Sigma}_{SS}$ were chosen using the unbiased risk estimate [8, Chapter 3.22] and leave-one-subject-out cross validation. Performance is similar under both criteria; for brevity, results under losoCV are omitted. Tuning parameter selection for the regularized versions of the sample covariance matrix was performed using cross validation; for detailed discussion, see [7].

In general, our estimator outperforms the alternative estimators, particularly when the underlying true covariance matrix does not satisfy the implicit structural assumptions motivating their construction. While the sample covariance matrix is an unbiased estimator of the unstructured covariance matrix, the smoothing spline estimator is better for every simulation model, and the difference is larger as p increases. The smoothing spline estimator performs most poorly on Model III, where ϕ does not belong to the tensor product smoothing spline model space due to its discontinuous first derivative. Overall, the results indicate that the smoothing spline estimator achieves what it was designed to do; it provides a more stable estimate than the sample covariance matrix, but is guaranteed to be positive-definite unlike the soft thresholding estimator and the tapering estimator. It achieves this stability with added flexibility over the polynomial estimator.

		p	$\hat{\Sigma}_{oracle}$	$\hat{\Sigma}_{SS}$	$\hat{\Sigma}_{poly}$	S	S^{ω}	S^{λ}
Model I	$N = 50$	10	0.0135	0.0685	0.1102	1.2047	0.5369	1.1742
		20	0.0229	0.0834	0.1096	4.9850	1.3957	4.7796
		30	0.0196	0.1102	0.1127	12.5517	2.8019	11.3175
	$N = 100$	10	0.0105	0.0451	0.0531	0.5685	0.2045	0.5236
		20	0.0105	0.0425	0.0512	2.2831	0.5724	2.1358
		30	0.0139	0.0431	0.0472	5.2770	1.2430	4.9126
Model II	$N = 50$	10	0.0581	0.0689	4.7673	1.2832	1.4644	1.1770
		20	0.0439	0.0581	97.2334	5.1665	21.6407	39.3522
		30	0.0627	0.0811	153.9665	12.3582	55.3674	133.9980
	$N = 100$	10	0.0386	0.0457	4.7911	0.5812	0.8335	0.5628
		20	0.0269	0.0416	98.1989	2.3364	10.1841	10.0864
		30	0.0288	0.0367	158.2480	5.2389	33.5207	62.5030
Model III	$N = 50$	10	0.0619	0.3296	3.0108	1.2030	1.1460	1.1467
		20	0.0695	1.1100	62.7522	4.9824	17.2244	14.9189
		30	0.0576	2.3215	1091.1933	12.4792	49.9135	121.7795
	$N = 100$	10	0.0268	0.2904	3.0383	0.5699	0.5545	0.5371
		20	0.0275	1.1963	62.8960	2.2700	11.8274	9.5217
		30	0.0221	2.2811	1105.0449	5.2234	29.1693	60.3529
Model IV	$N = 50$	10	0.0217	0.3348	0.7144	1.2218	0.7397	1.1921
		20	0.0286	0.9177	1.4588	4.9091	1.9786	4.9206
		30	0.0283	1.5992	2.2173	12.6114	3.7440	12.1489
	$N = 100$	10	0.0125	0.3047	0.6958	0.5570	0.3168	0.5515
		20	0.0105	0.8911	1.4813	2.2659	0.9365	2.2474
		30	0.0134	1.5213	2.2228	5.2106	1.9312	5.2111
Model V	$N = 50$	10	0.0986	0.2769	1.2420	1.2023	18.5222	2.9824
		20	0.2512	0.7514	2.8557	5.0195	34.6618	13.8690
		30	0.2641	1.1776	4.5791	12.3460	46.5437	26.1364
	$N = 100$	10	0.0520	0.2416	1.1491	0.5821	16.4081	1.7397
		20	0.0827	0.7286	2.9080	2.2918	32.5295	5.4649
		30	0.1799	1.1813	4.4402	5.2197	39.2914	15.4295

Table 2: *Multivariate normal simulations for Model I - Model V. Estimated entropy risk is reported for the oracle estimator, our smoothing spline ANOVA estimator, the parametric polynomial estimator of Pan and MacKenzie (2003), the sample covariance matrix, the tapered sample covariance matrix, and the soft thresholding estimator.*

6. Data Analysis

[13] reported an experiment designed to investigate the impact of the control of intestinal parasites in cattle. To compare two methods for controlling the disease, say treatment A and treatment B, each of 60 cattle was assigned randomly to two groups, each of size 30. Animal subjects were put out to pasture at the start of grazing season, with each member of the groups receiving one of the two treatments. Animals were weighed 11 times

($p = 11$) over a 133-day period; the first 10 measurements on each animal were made at two-week intervals and the final measurement was made one week later. The longitudinal dataset is balanced, as there were no missing observations for any of the experimental units. Observed weights are shown in Figure 3.

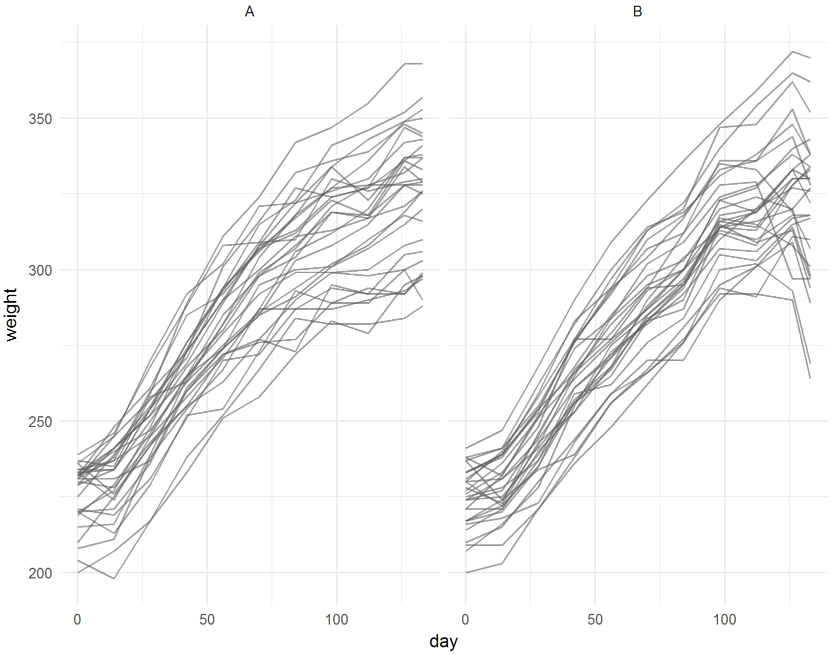


Figure 3: *Subject-specific weight curves over time for treatment groups A and B.*

The analysis of the same dataset provided by [32] rejected equality of the two covariance matrices corresponding to treatment group using the classical likelihood ratio test, making it reasonable to study each treatment group's covariance matrix separately. Following [18], [30], and [19], we analyze the data from the cattle assigned to treatment group A ($N = 30$). Given that the animals belong to the same treatment group and share a common set of observation times, we posit common covariance matrix Σ for each subject.

The left profile plot in Figure 3 of the weights for units in treatment group A shows a clear upward trend in weights. Variances appear to increase over time, suggesting that the covariance structure is nonstationary.

The nonstationarity suggested in Figure 3 is also supported by the sample correlations given in Table 3; correlations within the subdiagonals are not constant and increase over time, a secondary indication that a stationary covariance is not appropriate for the data.

						Day					
	0	14	28	42	56	70	84	98	112	126	133
0	1.00										
14	0.82	1.00									
28	0.76	0.91	1.00								
42	0.65	0.86	0.93	1.00							
56	0.63	0.83	0.89	0.93	1.00						
70	0.58	0.75	0.85	0.90	0.94	1.00					
84	0.51	0.64	0.75	0.80	0.85	0.92	1.00				
98	0.52	0.68	0.77	0.82	0.88	0.93	0.92	1.00			
112	0.51	0.61	0.71	0.74	0.81	0.89	0.92	0.96	1.00		
120	0.46	0.59	0.69	0.70	0.77	0.85	0.86	0.94	0.96	1.00	
133	0.46	0.56	0.67	0.67	0.74	0.81	0.84	0.91	0.95	0.98	1.00

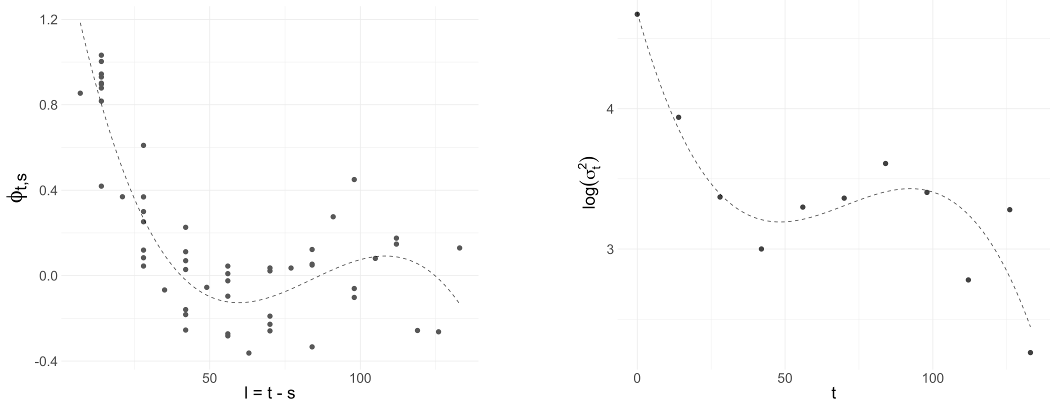
Table 3: *Cattle data: treatment group A sample correlations.*

As evident in Figure 3 with a trend in the observed weight trajectories, covariance estimation generally involves simultaneous modeling of mean trajectories. We adopt an approach akin to the dynamical conditionally linear mixed model presented in [22] and model the observed trajectory for the i^{th} subject, Y_i, as

$$Y_i = f\left(\mathcal{T}_i\right) + \alpha_i 1_{p_i} + \epsilon_i^*, \quad i = 1, \ldots, N, \tag{15}$$

where $f\left(\mathcal{T}_i\right) = \left(f(t_{i1}), \cdots, f(t_{i,p_i})\right)'$ is a vector of evaluation of a smooth function $f(t)$ that is common across the subjects at observed time points, and α_i is a random intercept corresponding to a subject-specific shift. For the cattle data, $\mathcal{T}_i = \{t_1 = 0, t_2 = 14, \cdots, t_{11} = 133\}$ same across the subjects. We assume that the random intercepts are independent and identically distributed with $N\left(0, \sigma_\alpha^2\right)$ and mutually independent of the measurement errors, ϵ_i^* that follow $N\left(0, \Sigma\right)$. These modeling assumptions allow us to estimate f with smoothing methods and the random intercepts based on the joint likelihood of f and α_i.

Analyzing the sample regressogram and sample innovation variogram, [19] suggested that both sample generalized autoregressive parameters and the logarithms of the innovation variances can be characterized in terms of cubic functions of the lag only and time, respectively. Figure 4 shows the estimated cubic polynomials according to the suggested model using the detrended trajectories with estimated means.



(a) *Sample generalized autoregressive parameters* $\hat{\phi}_{t,s}$.

(b) *Sample log innovation variances.*

Figure 4: *Cubic polynomomials fitted to the sample regressogram and log innovation variances for the cattle data from treatment group A.*

To model the mean weight trajectories, we adopt an approach akin to the dynamical conditionally linear mixed model presented in [22]:

$$Y_i = f\left(t_i\right) + Z_i b_i + \epsilon_i^*, \quad i = 1, \ldots, N, \tag{16}$$

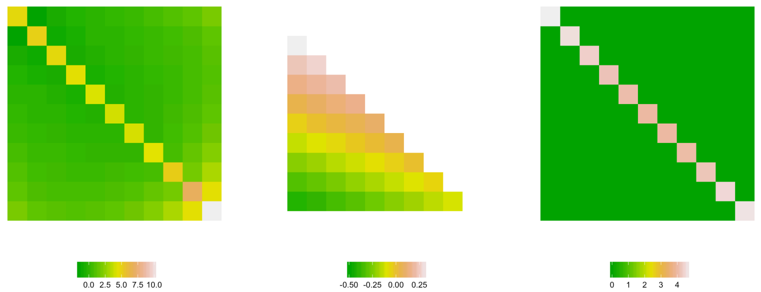
where Y_i is the measurement corresponding to response vector for the i^{th} subject, b_i is a $q \times 1$ vector of unknown random effects parameters, and Z_i is a known $p_i \times q$ design matrix. f is the smooth function of t, and $t_i = \left(t_{i1}, \ldots, t_{i,p_i}\right)'$ is the $p_i \times 1$ vector of measurement times for subject i. We take $Z_i = \left(1, \ldots, 1\right)'$ so that the random effects α_i correspond to subject-specific shifts. We assume to that the random intercepts are independent and identically distributed $N\left(0, \sigma_\alpha^2\right)$. We assume that the $p_i \times 1$ vector of residuals $\epsilon_i^* \sim N\left(0, \Sigma_i\right)$ are mutually independent of the random intercepts α_i. Given that the animals belong to the same treatment group and share a common set of observation times, we assume each subject shares common covariance matrix $\Sigma_i = \Sigma$.

Using cubic smoothing splines and the curvature penalty, we take the estimators of f, $\alpha = \left(\alpha_1, \ldots, \alpha_N\right)'$ to minimize the penalized joint log likelihood

$$\sum_{i=1}^{N}\sum_{i=1}^{p_i}\left(y_{ij} - f\left(t_{ij}\right) - \alpha_i\right)^2 + \alpha'\Sigma_\alpha^{-1}\alpha + \lambda J\left(f\right), \tag{17}$$

[18] had the same observation that the regressogram of empirical estimates of $\tilde{\phi}_{t,s}$ show consistent behaviour over $l = t - s$ for each value of t, indicating a lack of a strong functional component of m. This is consistent Pourahmadi's choice [**?**]see¿wu2003nonparametric in the specification of model the generalized autoregressive coefficients ϕ_{tj} in terms of lag only.

To balance the consideration of previous analyses with the interest of entirely data-driven model specification, we take our approach to estimation of the autoregressive coefficient function ϕ using a two-way ANOVA model in a tensor product space $\mathcal{H} = \mathcal{H}^{[l]} \otimes \mathcal{H}^{[m]}$, where penalties for $\mathcal{H}^{[l]}$ and $\mathcal{H}^{[m]}$ are specified to induce cubic splines and linear splines, respectively. Figure 5 shows the estimated covariance matrix, Cholesky surface and innovation variance function evaluated at pairs of observation times. The ANOVA decomposition of $\hat{\phi}$ into the functional components is shown in Figure 6.



(a) $\hat{\Sigma} = \hat{T}^{-1}\hat{D}\hat{T}'^{-1}$ (b) $\hat{\phi}\left(t, s\right)$ (c) $\log\hat{\sigma}^2\left(t\right)$

Figure 5: *The estimated covariance matrix for the cattle weight data from treatment group A in panel (a) and the corresponding estimated components of the Cholesky decomposition in (b) and (c). The generalized autoregressive coefficient function* $\phi\left(t, s\right)$ *and the log innovation variances* $\log\sigma^2\left(t\right)$ *were estimated using a tensor product cubic spline and cubic spline, respectively.*

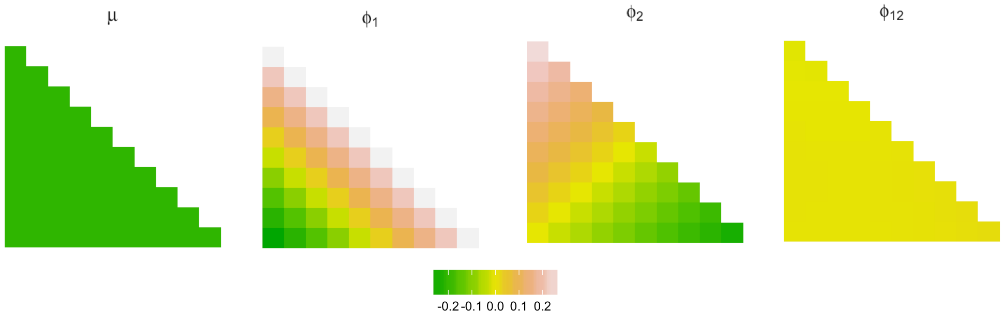


Figure 6: *Components of the two-way ANOVA decomposition of the estimated generalized autoregressive coefficient function ϕ evaluated on the grid defined by the observed time points. Displayed from left to right are the estimated overall mean ($\hat{\mu}$), main effect of lag ($\hat{\phi}_1$) and main effect of additive direction ($\hat{\phi}_2$) and their interaction ($\hat{\phi}_{12}$).*

The size of the functional components (in terms of the squared functional norm) indicates a certain degree of concordance with the models proposed by [19]. The squared norm of the main effect of lag (1.914) is over twice that of the main effect of additive direction (0.790). The squared norm of the interaction term, as clearly indicated by Figure 6, is negligible in comparison to the main effects, which suggests that parameterizing ϕ as a univariate function of lag only is a reasonable modeling choice.

7. Conclusions

We have proposed a general nonparametric framework for longitudinal data covariance estimation. The Cholesky decomposition supplies a reparameterization of the covariance matrix allowing for unconstrained estimation. The elements of the reparameterization can be interpreted as parameters for an autoregressive model. We allow for irregular, subject-specific time points by extending this regression model to a functional varying coefficient model. By reframing covariance estimation as the estimation of the functional varying coefficient function and the error variance function, our approach leverages regularization techniques that are typically reserved for function estimation. A functional ANOVA model leads to an interpretable decomposition of the varying coefficient into its stationary and non-stationary functional components. This parameterization naturally allows for shrinkage of estimated covariances toward those corresponding to stationary models.

In the standard function estimation setting, penalized likelihood estimation in a reproducing kernel Hilbert space with square semi norm defined by a penalty functional J is equivalent to specifying a certain empirical Bayes model with Gaussian prior with parameters corresponding to the smoothing parameters associated with the penalty term. See [8, Chapter 3.3]. A good choice of penalty functional is of key importance in penalized regression; however, in practice, penalty specification is often based on expert knowledge about the underlying generating mechanism of the data. In the context of smoothing spline models for covariance estimation, there may be more than one sensible choice for the penalties on ϕ and $\log \sigma^2$, and the optimal choice may not be obvious. In an unpublished manuscript, [31] propose adopting a Bayesian perspective which takes all candidate penalties into consideration. They propose a mixture distribution as a prior for the smoothing parameters to model uncertainty in the choice of penalty. Their perspective presents a potential way of choosing the appropriate class of null models for the varying coefficient function defining the Cholesky factor in a data-driven manner.

8. Acknowledgements

This research was supported in part by the National Science Foundation under grant DMS-15-13566.

9. Appendix

Theorem 1. The function space $\mathcal{H}$ is decomposed into $\mathcal{H}_0$ and $\mathcal{H}_1$. $\mathcal{H}_1$ can be further decomposed into the finite dimensional subspace spanned by $\{K_1(\boldsymbol{v}_j, \boldsymbol{v})\}$, $j = 1, \ldots, |V|$ and its orthogonal complement in $\mathcal{H}_1$. Considering the three subspaces, any $\phi \in \mathcal{H}$ can be written as

$$\phi(\boldsymbol{v}) = \sum_{i=1}^{\mathcal{N}_0} d_i \nu_i(\boldsymbol{v}) + \sum_{\boldsymbol{v}_j \in V} c_j K_1(\boldsymbol{v}_j, \boldsymbol{v}) + \rho(\boldsymbol{v}), \tag{18}$$

where $\rho \in \mathcal{H}_1$ is perpendicular to $\nu_1, \ldots, \nu_{\mathcal{N}_0}$ and $K_1(\boldsymbol{v}_j, \boldsymbol{v})$ for $\boldsymbol{v}_j \in V$.

Using the properties of the reproducing kernel $K = K_0 + K_1$, we can show that evaluation of any $\phi \in \mathcal{H}$ at $\boldsymbol{v}_\ell \in V$ does not depend on ρ:

$$\begin{aligned}
\phi(\boldsymbol{v}_\ell) &= \langle \phi(\cdot), K(\boldsymbol{v}_\ell, \cdot) \rangle_{\mathcal{H}} \\
&= \langle \sum_{i=1}^{\mathcal{N}_0} d_i \nu_i(\cdot) + \sum_{\boldsymbol{v}_j \in V} c_j K_1(\boldsymbol{v}_j, \cdot) + \rho(\cdot), K(\boldsymbol{v}_\ell, \cdot) \rangle_{\mathcal{H}} \\
&= \langle \sum_{i=1}^{\mathcal{N}_0} d_i \nu_i(\cdot) + \sum_{\boldsymbol{v}_j \in V} c_j K_1(\boldsymbol{v}_j, \cdot) + \rho(\cdot), K_0(\boldsymbol{v}_\ell, \cdot) \rangle_{\mathcal{H}} \\
&\qquad + \langle \sum_{i=1}^{\mathcal{N}_0} d_i \nu_i(\cdot) + \sum_{\boldsymbol{v}_j \in V} c_j K_1(\boldsymbol{v}_j, \cdot) + \rho(\cdot), K_1(\boldsymbol{v}_\ell, \cdot) \rangle_{\mathcal{H}} \\
&= \langle \sum_{i=1}^{\mathcal{N}_0} d_i \nu_i(\cdot), K_0(\boldsymbol{v}_\ell, \cdot) \rangle_{\mathcal{H}} + \langle \sum_{\boldsymbol{v}_j \in V} c_j K_1(\boldsymbol{v}_j, \cdot), K_0(\boldsymbol{v}_\ell, \cdot) \rangle_{\mathcal{H}} + \langle \rho(\cdot), K_0(\boldsymbol{v}_\ell, \cdot) \rangle_{\mathcal{H}} \\
&\quad + \langle \sum_{i=1}^{\mathcal{N}_0} d_i \nu_i(\cdot), K_1(\boldsymbol{v}_\ell, \cdot) \rangle_{\mathcal{H}} + \langle \sum_{\boldsymbol{v}_j \in V} c_j K_1(\boldsymbol{v}_j, \cdot), K_1(\boldsymbol{v}_\ell, \cdot) \rangle_{\mathcal{H}} + \langle \rho(\cdot), K_1(\boldsymbol{v}_\ell, \cdot) \rangle_{\mathcal{H}} \\
&= \langle \sum_{i=1}^{\mathcal{N}_0} d_i \nu_i(\cdot), K_0(\boldsymbol{v}_\ell, \cdot) \rangle_{\mathcal{H}} + \langle \sum_{\boldsymbol{v}_j \in V} c_j K_1(\boldsymbol{v}_j, \cdot), K_1(\boldsymbol{v}_\ell, \cdot) \rangle_{\mathcal{H}} \\
&= \sum_{i=1}^{\mathcal{N}_0} d_i \nu_i(\boldsymbol{v}_\ell) + \sum_{\boldsymbol{v}_j \in V} c_j K_1(\boldsymbol{v}_j, \boldsymbol{v}_\ell).
\end{aligned}$$

The last two equalities result from the orthogonality of $\mathcal{H}_0$, $\{K_1(\boldsymbol{v}_j, \boldsymbol{v})\}$, and ρ, and the reproducing property of K. Thus, the negative log likelihood in (7) depends only on $\sum_{i=1}^{\mathcal{N}_0} d_i \nu_i(\boldsymbol{v}) + \sum_{\boldsymbol{v}_j \in V} c_j K_1(\boldsymbol{v}_j, \boldsymbol{v})$. On the other hand, the penalty is given by

$$\begin{aligned}
||P_1 \phi||^2 &= || \sum_{\boldsymbol{v}_j \in V} c_j K_1(\boldsymbol{v}_j, \cdot) + \rho(\cdot) ||_{\mathcal{H}}^2, \\
&= || \sum_{\boldsymbol{v}_j \in V} c_j K_1(\boldsymbol{v}_j, \cdot) ||_{\mathcal{H}}^2 + || \rho(\cdot) ||_{\mathcal{H}}^2.
\end{aligned}$$

The penalized negative log likelihood is obviously minimized when $||\rho||^2 = 0$, or $\rho(\cdot) = 0$. This leads to the form of the minimizer for ϕ_λ as stated in Theorem 1. □

References

[1] Anderson, T. W., Anderson, T. W., Anderson, T. W., Anderson, T. W., and Mathématicien, E.-U. An introduction to multivariate statistical analysis, vol. 2. Wiley New York, 1958.

[2] Aronszajn, N. Theory of reproducing kernels. Transactions of the American Mathematical Society 68, 3 (1950), 337–404.

[3] Berlinet, A., and Thomas-Agnan, C. Reproducing kernel Hilbert spaces in probability and statistics. Springer Science & Business Media, 2011.

[4] Bickel, P. J., Levina, E., et al. Regularized estimation of large covariance matrices. The Annals of Statistics 36, 1 (2008), 199–227.

[5] Cai, T. T., Zhang, C.-H., Zhou, H. H., et al. Optimal rates of convergence for covariance matrix estimation. The Annals of Statistics 38, 4 (2010), 2118–2144.

[6] Eilers, P. H., and Marx, B. D. Flexible smoothing with b-splines and penalties. Statistical science (1996), 89–102.

[7] Fang, Y., Wang, B., and Feng, Y. Tuning-parameter selection in regularized estimations of large covariance matrices. Journal of Statistical Computation and Simulation 86, 3 (2016), 494–509.

[8] Gu, C. Smoothing spline ANOVA models, vol. 297. Springer Science & Business Media, 2013.

[9] Gu, C., and Wahba, G. Minimizing GCV/GML scores with multiple smoothing parameters via the newton method. SIAM Journal on Scientific and Statistical Computing 12, 2 (1991), 383–398.

[10] Huang, J. Z., Liu, L., and Liu, N. Estimation of large covariance matrices of longitudinal data with basis function approximations. Journal of Computational and Graphical Statistics 16, 1 (2007), 189–209.

[11] Huang, J. Z., Liu, N., Pourahmadi, M., and Liu, L. Covariance matrix selection and estimation via penalised normal likelihood. Biometrika (2006), 85–98.

[12] Johnstone, I. M. On the distribution of the largest eigenvalue in principal components analysis. Annals of Statistics (2001), 295–327.

[13] Kenward, M. G. A method for comparing profiles of repeated measurements. Applied Statistics (1987), 296–308.

[14] Leng, C., Zhang, W., and Pan, J. Semiparametric mean–covariance regression analysis for longitudinal data. Journal of the American Statistical Association 105, 489 (2010), 181–193.

[15] Levina, E., Rothman, A., and Zhu, J. Sparse estimation of large covariance matrices via a nested lasso penalty. The Annals of Applied Statistics (2008), 245–263.

[16] LIU, A., AND WANG, Y. Hypothesis testing in smoothing spline models. Journal of Statistical Computation and Simulation 74, 8 (2004), 581–597.

[17] PAN, J., AND MACKENZIE, G. On modelling mean-covariance structures in longitudinal studies. Biometrika 90, 1 (2003), 239–244.

[18] PAN, J., AND PAN, Y. Jmcm: An r package for joint mean-covariance modeling of longitudinal data. Journal of Statistical Software 82, 1 (2017), 1–29.

[19] POURAHMADI, M. Joint mean-covariance models with applications to longitudinal data: Unconstrained parameterisation. Biometrika 86, 3 (1999), 677–690.

[20] POURAHMADI, M. Maximum likelihood estimation of generalised linear models for multivariate normal covariance matrix. Biometrika (2000), 425–435.

[21] POURAHMADI, M. Covariance estimation: The GLM and regularization perspectives. Statistical Science (2011), 369–387.

[22] POURAHMADI, M., AND DANIELS, M. Dynamic conditionally linear mixed models for longitudinal data. Biometrics 58, 1 (2002), 225–231.

[23] ROTHMAN, A. J., LEVINA, E., AND ZHU, J. Generalized thresholding of large covariance matrices. Journal of the American Statistical Association 104, 485 (2009), 177–186.

[24] WAHBA, G. Spline models for observational data, vol. 59. Siam, 1990.

[25] WAHBA, G., WANG, Y., GU, C., KLEIN, R., AND KLEIN, B. Smoothing spline anova for exponential families, with application to the wisconsin epidemiological study of diabetic retinopathy. The Annals of Statistics (1995), 1865–1895.

[26] WANG, Y. Grkpack fitting smoothing spline anova models for exponential families. Communications in Statistics-Simulation and Computation 26, 2 (1997), 765–782.

[27] WU, W. B., AND POURAHMADI, M. Nonparametric estimation of large covariance matrices of longitudinal data. Biometrika 90, 4 (2003), 831–844.

[28] XU, G., HUANG, J. Z., ET AL. Asymptotic optimality and efficient computation of the leave-subject-out cross-validation. The Annals of Statistics 40, 6 (2012), 3003–3030.

[29] YAO, F., MÜLLER, H.-G., AND WANG, J.-L. Functional data analysis for sparse longitudinal data. Journal of the American Statistical Association 100, 470 (2005), 577–590.

[30] ZHANG, W., LENG, C., AND TANG, C. Y. A joint modelling approach for longitudinal studies. Journal of the Royal Statistical Society: Series B (Statistical Methodology) 77, 1 (2015), 219–238.

[31] ZHANG, X., DATTA, G. S., MA, P., AND ZHONG, W. Bayesian spline smoothing with ambiguous penalties. Presented at the 2018 Joint Statistical Meetings, Vancouver, British Columbia, 2018.

[32] ZIMMERMAN, D. L., AND NÚÑEZ-ANTÓN, V. Structured antedependence models for longitudinal data. In Modelling longitudinal and spatially correlated data. Springer, 1997, pp. 63–76.