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Conditional Gaussian Graphical Models for Functional Variables with Partially Separable Operators

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Abstract

Functional graphical modeling is gaining increasing attention in recent years. In this paper, we contribute to the literature by extending the notion of conditional Gaussian graphical model to a functional setting. We propose a double-penalized estimator and an efficient algorithm to recover the edge-set encoding both the conditional covariance structure of the response functions and the effects of the predictor functions on the conditional distribution.

Keywords: Graphical models, multivariate functional data, multivariate Gaussian process, partial separability, sparse inference.

1. Introduction

In recent years, functional data has become a commonly encountered data type. The first approach aimed to extend graphical models to the functional setting was proposed in (6), where, under the assumption that the random functions follow a multivariate Gaussian process (MGP), the authors introduce the notion of functional Gaussian graphical model (fGGM) and an extension of the graphical lasso (glasso) (9) to estimate the edge-set encoding the conditional dependence structure. A notion of conditional functional graphical model, where the graph links are allowed to vary with the external variables, is introduced in (5). In this paper, we are not interested in constructing a random graph; rather, we are interested in the effect of the explanatory variables on the expected value of the multivariate response process. Recently, in (10) is addressed the general problem of covariance modelling for multivariate functional data, particularly fGGMs. The authors introduce the notion of partial separability for the covariance operator and show that this is particularly useful in functional graphical modelling (FGM) since it allows us to overcome the theoretical problems related to the covariance operator, which is compact and thus not invertible.

In this paper, we contribute to the literature on FGM by extending the notion of conditional Gaussian graphical model (cGGM) (8) and proposing a double-penalized estimator by which to recover the edge-set of the corresponding graph. We complete this section by providing a brief description of the cGGM models.

Let $\boldsymbol{X} = (X_1, \ldots, X_q)^\top$ and $\boldsymbol{Y} = (Y_1, \ldots, Y_p)^\top$ be two random vectors. cGGMs are based on the assumption that $\boldsymbol{Y} \mid \boldsymbol{x} \sim N(\boldsymbol{Bx}, \Sigma)$, where $\boldsymbol{Bx} = \mathrm{E}(\boldsymbol{Y} \mid \boldsymbol{x})$ and $\Sigma = \mathrm{V}(\boldsymbol{Y} \mid \boldsymbol{x})$, and that exists a graph $\mathscr{G} = (\mathscr{V}, \mathscr{E} = \mathscr{E}_\mu \cup \mathscr{E}_\Theta)$ encoding the effects of $\boldsymbol{X}$ onto the conditional distribution of $\boldsymbol{Y}$. The edge-set $\mathscr{E}$ is defined as the union of two specific sets. The set $\mathscr{E}_\mu$ contains the directed links representing the effects of $\boldsymbol{X}$ on $\mathrm{E}(\boldsymbol{Y} \mid \boldsymbol{x})$, i.e., the directed link (m,h) belongs to $\mathscr{E}_\mu$ iff X_m has an effect on the conditional expected value of Y_h, i.e., $\beta_{hm} \neq 0$. The set $\mathscr{E}_\Theta$ contains the undirected links depicting the conditional dependence structure among the response variables, consequently, according to the standard theory on the factorization of the multivariate Gaussian distribution (see (4) for more details), the undirected link (h,k) belongs to $\mathscr{E}_\Theta$ iff the corresponding element of the precision matrix $\Theta = \Sigma^{-1}$ is different from zero. In this class of graphical models, our final goal is to estimate $\boldsymbol{B}$ and Θ and recover the information encoded in $\mathscr{E}$.

2. The functional conditional Gaussian graphical model

Notation We use the term multivariate functional data to refer to the realization of a multivariate process. Specifically, we denote the multivariate processes corresponding to the response and predictor functions as $\mathscr{P}_Y = \{\boldsymbol{\mathscr{Y}}(t) \in \mathbb{R}^p : t \in \mathscr{T}\}$ and $\mathscr{P}_X = \{\boldsymbol{\mathscr{X}}(s) \in \mathbb{R}^q : s \in \mathscr{S}\}$, where $\mathscr{T}$ and $\mathscr{S}$ are closed subsets of $\mathbb{R}$. It is assumed that $\mathscr{P}_Y$ and $\mathscr{P}_X$ are MGPs and that $\mathscr{Y}_h$ and $\mathscr{X}_m$ are elements of $\mathscr{L}_2(\mathscr{T})$ and $\mathscr{L}_2(\mathscr{S})$, where $\mathscr{L}_2(\cdot)$ denotes the Hilbert space of square-integrable functions endowed with the standard inner product $\langle g_1, g_2 \rangle = \int_{\mathscr{S}} g_1(s) g_2(s) ds$ and norm $\|\cdot\| = \langle \cdot, \cdot \rangle^{1/2}$. We also assume that $\boldsymbol{\mathscr{X}}$ has zero mean and a smooth covariance function $G^X(s_1,s_2) = \{G^X_{mn}(s_1,s_2)\}$, where $G^X_{mn}(s_1,s_2) = \mathrm{cov}(\mathscr{X}_m(s_1), \mathscr{X}_n(s_2))$. Similarly, $\boldsymbol{\mathscr{Y}}$ has zero mean and smooth covariance function $G^Y(t_1,t_2) = \{G^Y_{hk}(t_1,t_2)\}$. Finally, for each bivariate function $f \in \mathscr{L}_2(\mathscr{T} \times \mathscr{S})$, by $\|f\| = \{\int\int f(t,s) dt ds\}^{1/2}$ we denote the Hilbert-Schimdt norm.

The functional conditional Gaussian graphical model We are interesting in inferring how the predictor process affects the distribution of the conditional process $\mathscr{P}_{Y|X} = \{\boldsymbol{\mathscr{Y}}(t) \mid \boldsymbol{\mathscr{X}} : t \in \mathscr{T}\}$, which is Gaussian and uniquely specified by:

$$\mathrm{E}(\mathscr{Y}_h(t) \mid \boldsymbol{\mathscr{X}}) = \sum_{m=1}^{q} \int_{\mathscr{S}} \beta_{hm}(t,s) \mathscr{X}_m(s) ds, \quad G^{Y|X}(t_1,t_2) = \left\{ G^{Y|X}_{hk}(t_1,t_2) \right\}, \tag{1}$$

where $\beta_{hm}(t,s) \in \mathscr{L}_2(\mathscr{T} \times \mathscr{S})$ are the bivariate regression coefficient functions, and $G^{Y|X}_{hk}(t_1,t_2) = \mathrm{cov}(\mathscr{Y}_h(t_1), \mathscr{Y}_k(t_2) \mid \boldsymbol{\mathscr{X}})$ is the conditional covariance function. To provide a coherent extension of the cGGM, we must define the edge-sets $\mathscr{E}_\mu$ and $\mathscr{E}_\Theta$. While the first set can be easily defined using the left-hand-side in (1), i.e., $\mathscr{E}_\mu = \{(m,h) : \|\beta_{hm}\| \neq 0\}$, a proper definition of $\mathscr{E}_\Theta$ can be obtained only through the notion of conditional cross-covariance function (6):

$$C^{Y|X}_{hk}(t_1,t_2) = \mathrm{cov}(\mathscr{Y}_h(t_1), \mathscr{Y}_k(t_2) \mid \boldsymbol{\mathscr{Y}}_{-(hk)}, \boldsymbol{\mathscr{X}}), \tag{2}$$

which represents the covariance between $\mathscr{Y}_h$ and $\mathscr{Y}_k$ given the processes $\boldsymbol{\mathscr{Y}}_{-(hk)}$ and $\boldsymbol{\mathscr{X}}$. Using (2), we define $\mathscr{E}_\Theta = \{(h,k) : \|C^{Y|X}_{hk}\| \neq 0\}$. In the remaining part of this paper, by functional conditional Gaussian graphical model (fcGGM) we mean the set $\{\mathscr{P}_{Y|X}, \mathscr{G} = \{\mathscr{V}, \mathscr{E} = \mathscr{E}_\mu \cup \mathscr{E}_\Theta\}\}$, and our goal is to recover the edge-set $\mathscr{E}$.

Partial separability and fcGGM In principle, we could recover $\mathscr{E}$ using the approach presented in (6), representing each random function by the coefficients of a truncated basis expansion and then estimating $\mathscr{E}$ using a modified glasso estimator. Although this method is an intuitive approach to FGM estimation, the authors show the existence of a theoretical link between precision matrix and true FGM, only under the assumption that each random function takes values in a finite-dimensional space. As elucidated in (10), in an infinite-dimensional setting, the relationship between precision matrix and conditional independence structure is lost because the covariance operator is compact and thus not invertible; therefore, to estimate $\mathscr{E}$ in an fcGGM, we enforce our assumptions by assuming that the covariance operators G^X and G^Y are partially separable. As a consequence, by Theorem 1 in (10), we have the following multivariate expansions:

$$\mathscr{Y}_h(t) = \sum_{l=1}^{+\infty} Y_{hl}\varphi_l(t), \quad \text{and} \quad \mathscr{X}_m(s) = \sum_{l=1}^{+\infty} X_{ml}\psi_l(s), \tag{3}$$

where $\{\varphi_l\}_{l=1}^{+\infty}$, $\{\psi_l\}_{l=1}^{+\infty}$ are orthonormal bases of $\mathscr{L}_2(\mathscr{T})$ and $\mathscr{L}_2(\mathscr{S})$, whereas $Y_{hl} = \langle \mathscr{Y}_h, \varphi_l \rangle$, $X_{ml} = \langle \mathscr{X}_m, \phi_l \rangle$ are random variables. Since $\mathscr{P}_Y$ and $\mathscr{P}_X$ are Gaussian, the vector $\boldsymbol{Z}_l = (X_{1l},\ldots,X_{ql},Y_{1l},\ldots,Y_{pl})^\top$ is also Gaussian with parameters, $\mathrm{E}(\boldsymbol{Z}_l) = \boldsymbol{0}$ and $V(\boldsymbol{Z}_l) = \Sigma_l$. Moreover, $\boldsymbol{Z}_l \perp\!\!\!\perp \boldsymbol{Z}_{l'}$. Using (3), it is possible to show that:

$$\mathrm{E}(\mathscr{Y}_h(t) \mid \boldsymbol{\mathscr{X}}) = \sum_{m=1}^{q}\sum_{l=1}^{+\infty} \beta_{hml} x_{ml} \varphi_l(t), \tag{4}$$

where x_{ml} denotes a realization of X_{ml} and $\sum_{m=1}^{q} \beta_{hml} x_{ml} = \mathrm{E}(Y_{hl} \mid \boldsymbol{X}_l)$. A direct consequence of the expansion (4) is that $\mathscr{E}_\mu$ can be defined in terms of β_{hml}, i.e., $(m,h) \in \mathscr{E}_\mu$ iff exists at least an index $l \in \mathbb{N}$ such that $\beta_{hml} \neq 0$.

The main advantage of the expansion (4) is that it allows us to express the conditional cross-covariance function (2) in terms of conditional covariance between Y_{hl} and Y_{kl}. First, note that expansion (4) also implies that the residual process admits a multivariate expansion of type (3), thus, according to Theorem 1 of (10), the covariance operator in (1) is also partially separable, consequently, using Theorem 3 in (10) and the standard results on the conditional Gaussian distribution, we have:

$$C_{hk}^{Y|X}(t_1,t_2) = \sum_{l=1}^{+\infty} \mathrm{cov}(Y_{hl}, Y_{kl} \mid \boldsymbol{Y}_{-(hk)}, \boldsymbol{X}_l)\varphi_l(t_1)\varphi_l(t_2) = -\sum_{l=1}^{+\infty} \frac{\theta_{hkl}\varphi_l(t_1)\varphi_l(t_2)}{\theta_{hhl}\theta_{kkl} - \theta_{hkl}^2}, \tag{5}$$

where θ_{hkl} are the entries of $\Theta_l = \mathrm{V}(\boldsymbol{Y}_l \mid \boldsymbol{X}_l)^{-1}$. Using (5) it follows that an undirected link, say (h,k), belongs to $\mathscr{E}_\Theta$ iff exists at least an index $l \in \mathbb{N}$ such that $\theta_{hkl} \neq 0$.

The functional joint conditional graphical lasso estimator In the previous section, we have shown that all the necessary information needed to recover the edge set associated with an fcGGM is contained in the conditional distribution of $\boldsymbol{Y}_l$ given $\boldsymbol{X}_l$. Below, we propose a two-step procedure to estimate $\mathscr{E}$.

Step 1. Suppose we observe N independent realizations from $\mathscr{P}_Y$ and $\mathscr{P}_X$, denoted by $\boldsymbol{\mathscr{Y}}_i = (\mathscr{Y}_{i1},\ldots,\mathscr{Y}_{ip})^\top$ and $\boldsymbol{\mathscr{X}}_i = (\mathscr{X}_{i1},\ldots,\mathscr{X}_{ip})^\top$, with $i = 1,\ldots,N$, over T time instants. Expansions (3) allow us to represent each random function as an infinite-dimensional object; thus, it is necessary for some form of dimensionality reduction. First, the mean functions are calculated over the observed time instants as $\bar{\mathscr{Y}}_h(t) = \sum_{i=1}^{N} \mathscr{Y}_{ih}(t)/N$. Then p autocovariance matrices are estimated and each entry is given by $[\widehat{G}_h^Y]_{1,2} = \sum_{i=1}^{N}\{\mathscr{Y}_{ih}(t_1) - \bar{\mathscr{Y}}_h(t_1)\}\{\mathscr{Y}_{ih}(t_2) - \bar{\mathscr{Y}}_h(t_2)\}/N$. All those $T \times T$ matrices are summed and divided by p in order to have $\widehat{H}^Y$, which indicates the mean-variance over the responses variables for each couple of time instants. According to Theorem 2 in (10), the basis functions $\varphi_l(t)$ can be estimated performing the eigen-decomposition on $\widehat{H}^Y$. Each $\mathscr{Y}_{ih}$ can be approximated using the first L leading terms, i.e., the function $\mathscr{Y}_{ih}^L(t) = \sum_{l=1}^{L} y_{ihl}\widehat{\varphi}_l(t)$, where the estimated principal component scores are $y_{ihl} = \langle \mathscr{Y}_{ih}, \widehat{\varphi}_l \rangle$. The procedure described above is used to estimate the quantities related to $\mathscr{X}_{im}(s)$, i.e., $\widehat{\psi}_l(s)$ and the corresponding scores $x_{iml} = \langle \mathscr{X}_{im}, \widehat{\psi}_l \rangle$. For ease of notation, we suppose again to use the first L leading terms to approximate the random predictor functions, i.e., $\mathscr{X}_{im}^L(s) = \sum_{l=1}^{L} x_{iml}\widehat{\psi}_l(s)$.

Step 2. Let $\mathbf{Y}_l = (y_{ihl})$ and $\mathbf{X}_l = (x_{iml})$, with $l = 1,\ldots,L$, be the matrices of the estimated scores. Given the assumption underlying the fcGGM, the rows of these matrices are independent realizations from a multiple cGGM, i.e., a collection of cGGMs; therefore, the sets $\mathscr{E}_\mu$ and $\mathscr{E}_\Theta$ can be estimated using a proper extension of the joint glasso (2), such as the one proposed in (3) or, in the context of censored data, in (1) and (7).

Let us denote by $\boldsymbol{B}_l$ and Θ_l the parameters associated to the lth cGGM and let $\{\boldsymbol{B}\} = \{\boldsymbol{B}_1,\ldots,\boldsymbol{B}_L\}$ and $\{\Theta\} = \{\Theta_1,\ldots,\Theta_L\}$. As the assumption of partial separability implies that $\boldsymbol{Z}_l \perp\!\!\!\perp \boldsymbol{Z}_{l'}$, for each $l \neq l'$, we propose to recover $\mathscr{E}$ using the following double-penalized estimator, named functional joint conditional glasso estimator:

$$\{\widehat{\boldsymbol{B}}\}, \{\widehat{\Theta}\} = \arg\max \sum_{l=1}^{L} \{\log\det\Theta_l - \mathrm{tr}(\mathsf{S}(\boldsymbol{B}_l)\Theta_l)\} - \lambda P_1(\{\boldsymbol{B}\}) - \rho P_2(\{\Theta\}), \tag{6}$$

where $\mathsf{S}(\boldsymbol{B}_l) = (\mathsf{Y}_l - \mathsf{X}_l\boldsymbol{B}_l)^\top(\mathsf{Y}_l - \mathsf{X}_l\boldsymbol{B}_l)/N$. The penalty functions in (6) selects convex functions that encourage sparsity in each matrix and specific forms of similarity across the regression coefficient matrices and the precision matrices. In this paper, we propose to use the group lasso penalty functions: $P_1(\{\boldsymbol{B}\}) = \sum_{h=1}^{p}\sum_{m=1}^{q}\left(\sum_{l=1}^{L}\beta_{hml}^2\right)^{1/2}$ and $P_2(\{\Theta\}) = \sum_{h\neq k}\left(\sum_{l=1}^{L}\theta_{hkl}^2\right)^{1/2}$, thus, the desired edge-sets can be estimated by $\widehat{\mathscr{E}}_\mu = \left\{(m,h) : \sum_{l=1}^{L}\hat{\beta}_{hml}^2 > 0\right\}$ and $\widehat{\mathscr{E}}_\Theta = \left\{(h,k) : \sum_{l=1}^{L}\hat{\theta}_{hkl}^2 > 0\right\}$.

3. A simulation study

To simulate a sample of $N = 600$ independent observations from an fcGGM, we use the following model:

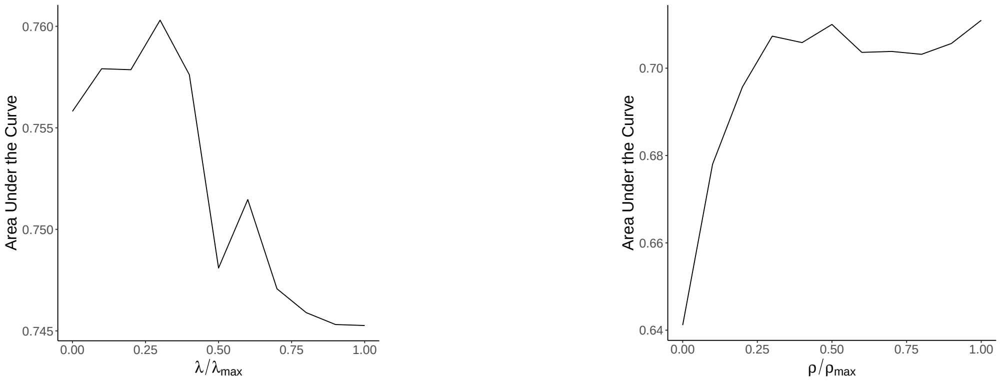
$$y_{ihr}^{L} = \sum_{l=1}^{L} y_{ihl}\varphi_l(t_r) + \varepsilon_{ihr}, \qquad x_{imr}^{L} = \sum_{l=1}^{L} x_{iml}\psi_l(s_r) + \varepsilon_{imr},$$

where ε_{ihr} and ε_{imr} are independent random errors drawn from $N(0,10)$, $\{t_r\}_{r=1}^{30}$ and $\{s_r\}_{r=1}^{30}$ are evenly spaced sequences with $t_1 = s_1 = 0$ and $t_{30} = s_{30} = 1$, and $\{\varphi_l\}, \{\psi_l\}$ are Fourier bases. In our study, we set $L = 3$, $p = 24$ and $q = 7$. According to the assumptions underlying the proposed fcGGM, for each l, the vectors $\boldsymbol{z}_{il} = (\boldsymbol{x}_{il}^\top, \boldsymbol{y}_{il}^\top)^\top$ are independent realizations from a multivariate Gaussian distribution with zero expected value and covariance matrix Σ_l^z structured as follows:

$$\Sigma_l^z = 3l^{-1.8} \times \begin{bmatrix} \sigma_x^2\boldsymbol{I} + \boldsymbol{B}_l\Theta_l\boldsymbol{B}_l^\top & -\boldsymbol{B}_l\Theta_l \\ -\Theta_l\boldsymbol{B}_l^\top & \Theta_l \end{bmatrix}^{-1}. \tag{7}$$

where, as in (10), the decreasing factor $3l^{1.8}$ guarantees that $\mathrm{tr}(\Sigma_l^z)$ decreases monotonically in l, whereas the quantities in the matrix in (7) are related to the marginal distribution of $\boldsymbol{X}_{il}$ and to the conditional distribution of $\boldsymbol{Y}_{il}$ given $\boldsymbol{x}_{il}$ be the identities: $\mathrm{V}(\boldsymbol{X}_{il}) = \sigma_x^2\boldsymbol{I}$, with $\sigma_x^2 = 20$, $\mathrm{E}(\boldsymbol{Y}_{il} \mid \boldsymbol{x}_{il}) = \boldsymbol{B}_l\boldsymbol{x}_{il}$ and, finally, $\{\mathrm{V}(\boldsymbol{Y}_{il} \mid \boldsymbol{x}_{il})\}^{-1} = \Theta_l$. To generate a sparse fcGGM, for each l, each row of $\boldsymbol{B}_l$ has only two non-zero regression coefficients sampled from $U([-0.8,-0.5] \cup [+0.5,+0.8])$ whereas the conditional precision matrix Θ_l is structured in such a way that the associated graph is the union of a common and a specific star. Formally, the non-zero entries of each Θ_l are sampled by the model: $\theta_{hkl} \sim U([-0.15,-0.10] \cup [+0.10,+0.15])$, with $h \in \{1, 6l+1\}$ and $k = (h+1),\ldots,(h+5)$.

To compute the estimator (6), we use the algorithm proposed in (7). The behaviours of $\mathscr{E}_{\widehat{\Theta}}$ and $\mathscr{E}_{\hat{\mu}}$ are studied under different combinations of λ and ρ; to analyze the coefficient path for $\{\widehat{\Theta}\}$, we first control the amount of shrinkage on $\{\widehat{\boldsymbol{B}}\}$ by keeping fixed the ratio λ/λ_{max}, and then, for this fixed λ value, the path for $\{\widehat{\Theta}\}$ is computed across a decreasing sequence of eleven evenly spaced values of ρ, from ρ_{max} to 0 with steps equal to $0.1 \times \rho_{max}$. We use the median area under ROC curves to evaluate the resulting path in network recovery. Figure 1 shows the results. The left side of figure 1 shows the values of the AUC given by the eleven values of ρ when λ is fixed. On the $X-$axes, there is the value of λ expressed in percentage of its maximum value; the first value, $0 \times \lambda_{max}$, corresponds to the case in which $\{\widehat{\boldsymbol{B}}\}$ is not penalized, the last value corresponds to the case where the predictor variables do not affect the conditional expected value of the response variables. On the $Y-$axes, the AUC median value over 50 simulations with λ fixed is reported. The left side of figure 1 shows that the level of shrinkage of $\{\widehat{\boldsymbol{B}}\}$ affects the ratio between TPR and FPR of $\mathscr{E}_{\widehat{\Theta}}$, indeed, when the penalization for $\{\widehat{\boldsymbol{B}}\}$ is small, the resulting AUC of the network recovery for $\{\widehat{\Theta}\}$ is high. The higher the penalization parameter for $\{\widehat{\boldsymbol{B}}\}$, the more difficult for the model to detect the correct set of edges, suggesting that the explanatory variables are needed for an accurate evaluation of $\mathscr{E}_{\widehat{\Theta}}$ and that the regression model is working well. The comparison of $\{\widehat{\boldsymbol{B}}\}$ paths is made using the same strategy as for $\{\widehat{\Theta}\}$, but inverting the role. Unlike the



(a) AUC of $\{\widehat{\Theta}\}$

(b) AUC of $\{\widehat{\boldsymbol{B}}\}$

Figure 1: AUC for different percentages of λ_{max} and ρ_{max}, and different values of $\sigma_{\boldsymbol{x}}$.

plot on the left of figure 1, the plot on the right shows a light effect of ρ on the ROC curve for $\{\widehat{\boldsymbol{B}}\}$, which confirms what is known in the literature.

4. Conclusion

Our model employs the multivariate expansion proposed by (10), to decompose the variables into two components: the stochastic component, which does not depend on the continuous domain, and the deterministic component, which depends on the domain of the variables. To the best of our knowledge, the proposed model is the first in which the analysis of the stochastic component is used to infer the structure of the dependencies among variables on both the side of the conditional independence relations of the variables of a functional response process and their dependencies on the functional covariates. The simulation study shows good performance of the cfGGM in terms of adjacency regression and precision matrices.

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