Supervised Multiscale Dimension Reduction for Spatial Interaction Networks

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Abstract
We introduce a multiscale supervised dimension reduction method for SPatial Interaction Network (SPIN) data, which consist of a collection of interactions between units indexed by spatial coordinates. To facilitate regression analysis with SPIN predictors, we extend bag-of-words representations to more complex settings, in which each primitive variable being represented is essentially unique, so that it becomes necessary to group the variables in order to simplify the representation and enhance interpretability and statistical power. We propose an empirical Bayes approach called spinlets, which first constructs a partitioning tree to guide the reduction with mixed spatial granularities, and then refines the representation of predictors according to the relevance to the response. We consider an inverse Poisson regression model, regularized by a multiscale extension of the generalized double Pareto prior, induced via a novel tree-structured parameter expansion scheme. Our approach is motivated by an application in soccer analytics, in which we obtain spinlets visualizations of soccer passing networks under the supervision of team performance.

Keywords: generalized linear mixed model, multiresolution method, object data analysis, parameter expansion, spatial statistics, structured sparsity
1 Introduction

In modern applications, we frequently encounter complex object-type data, such as functions (Ramsay and Silverman, 2006), trees (Wang and Marron, 2007), shapes (Srivastava et al., 2011), and networks (Durante et al., 2017). In many instances, such data are collected repeatedly under different conditions, with an additional response variable of interest available for each replicate. This has motivated an increasingly rich literature on generalizing regression on vector predictors to settings involving more elaborate object-type predictors with special characteristics, such as functions (James, 2002), manifolds (Nilsson et al., 2007), tensors (Zhou et al., 2013), and undirected networks (Guha and Rodriguez, 2018).

Complex objects are often built recursively from simpler parts. In this article, we introduce a new class of object data, denoted composite objects (CO), which are structured data composed of primitive objects (POs). Many common data types can be seen as instances of the CO family, such as a collection of time-stamped events, connections between regions of the brain, or basketball shots on the court. The component POs in CO-type data can be enormous and mostly distinctive from one another across replicates, presenting new challenges for data exploration, analysis, and visualization.

We are interested in identifying the association between the patterns of coordinated interactions among individual units in a group and the performance of the group. In this article, we focus on analyzing the FIFA World Cup 2018 data collected by StatsBomb. In this dataset, we observe SPatial Interaction Networks (SPIN) data \( \mathcal{E}_i := \{e_k : k = 1, \ldots, q_i\} \) from replicate \( i \in \{1, \ldots, n\} \), which contains a collection of \( q_i \) completed passes. As illustrated in Figure 1, \( \mathcal{E}_i \) is in the CO form, with every constituent pass \( e_k \) viewed as a PO logged with the spatial locations of the passer and receiver. The associated response \( y_i \) may refer to a team performance metric such as goals scored or conceded, the number of shots on target, or other situational game factors.

We consider regression modeling with \( n \) observations of a scalar response \( y_i \) and a CO-valued predictor \( \mathcal{E}_i, i = 1, \ldots, n \). A primary challenge is to represent the CO data in a malleable form that facilitates multivariate analysis. In our motivating application, the dataset contains 50,159 completed passes with 49,988 unique locations of origin-destination in the 64 matches. One common practice is to divide \( \mathcal{P} := \bigcup_{i=1}^n \mathcal{E}_i \), the complete set of POs, into \( p \) non-overlapping subsets \( \mathcal{P} = \bigcup_{j=1}^m \Pi_j \) (with \( \Pi_j \cap \Pi_{j'} = \emptyset \) for \( j, j' \in \{1, \ldots, p\} \) and \( j \neq j' \)) through a predefined partitioning scheme \( \Pi = [\Pi_1, \ldots, \Pi_p] \). For example, Miller et al. (2014) discretizes the basketball court uniformly into tiles and counts the number of shots located in each tile. Durante et al. (2017) parcellates the brain into regions and investigates the network connectivity between pairs of regions. Under the partition \( \Pi \), the
\( \mathcal{E}_i \) can be represented as a \( p \)-dimensional count vector \( \mathbf{x}_i \in \mathbb{Z}^p \), where \( x_{i,j} = N(\mathcal{E}_i \cap \Pi_j) \) counts the occurrences of POs appearing in \( \mathcal{E}_i \) and belonging to subset \( \Pi_j \).

\[ \text{(a) 202 completed passes by France} \quad \text{(b) 448 completed passes by Croatia} \]

Figure 1: Spatial interaction networks in the 2018 FIFA World Cup Final (France 4-2 Croatia). The arrowed segments denote the pass from the location of passer to the location of receiver. Team’s direction of attack: from left to right.

This partition scheme inherently assumes the equivalence of the POs falling within the same group, and focuses on the variabilities in abundance across groups. At one extreme, the partition of singletons \( \{\{e\} : e \in \mathcal{P}\} \) treats all the unique POs as distinct, and thus induces a bag-of-words representation (Blei et al., 2003; Taddy, 2013). At the other extreme, the singleton partition \( \{\mathcal{P}\} \) treats all the POs as equivalent, and thus keeps only the information about sample size \( q_i \). As one can see, the choice of partitioning scheme and its scale will have a critical influence on inference.

Ideally, a reductive representation should promote the interpretability of the CO-type predictor and preserve the relevance to the response. However, such approaches are underdeveloped in the current literature. In this article, we propose spinlets—an adaptive multiscale representation for spatial interaction networks. The spinlets method uses the similarity among primitive objects for deriving a tree representation of the data.

Spinlets serves as a tool for visualization and statistical inference of SPIN data. In Figure 2, we plot three different types of reduced representations for the instances shown in Figure 1, based on (i) a predefined \( 3 \times 6 \) uniform parcellation of the pitch, (ii) a graph partitioning algorithm without supervision, and (iii) spinlets under the supervision of the number of goals scored. Each replicate is a unique team-game combination. Spinlets is
data-driven and can select multiple informative scales. As illustrated in Figure 2, the details of passing patterns in the backfield are coarsened.

![Figure 2: SPIN representation of France (first row) and Croatia (second row) in the 2018 World Cup Final. The colored arrows represent the grouped POs with width proportional to the count of occurrences in the group. For the sake of visualization, the origins (dashed) and destinations (solid) of the grouped POs are indicated by the convex hulls (shaded region) with the grouped POs located at the centroids of the polygons.](image)

There is a rich literature on supervised dimension reduction, covering LASSO (Tibshirani, 1996), supervised PCA (Bair et al., 2006; Barshan et al., 2011), and sufficient dimension reduction (SDR) methods, see Cook (2007), Adragni and Cook (2009) and the references cited therein. The reduction of complexity is typically achieved through variable selection or combination. Such approaches can accommodate vector predictors and perform well in high-dimensional settings; however, our application involves predictors with complex structures. SDR methods have been generalized to handle functional predictors (Ferré and Yao, 2003, 2005), matrix- or array-valued predictors (Li et al., 2010), and irregularly measured longitudinal predictors (Jiang et al., 2014). In this article, we center our focus on spatial networks as an instance of a composite data object.
There is a separate literature on multiscale geometric data representation, including diffusion maps (Lafon and Lee, 2006) and GMRA (Allard et al., 2012; Petralia et al., 2013). These approaches seek a reductive representation that reflects the intrinsic geometry of the high-dimensional data by partitioning the similarity graph of \( n \) data observations. In contrast, our spinlets method partitions the similarity graph of \( q = \sum_{i=1}^{n} q_i \) variables, with a different goal of identifying predictive groups of variables. Spinlets is similar in spirit with the treelets method (Lee et al., 2008), which organizes variables on a hierarchical cluster tree with multiscale bases; however, treelets is an unsupervised approach utilizing the sample correlation to construct the tree with a single cutoff height. Our spinlets approach departs from treelets by incorporating external proximity to construct the tree, and determining non-uniform heights (Meinshausen and Bühlmann, 2008) with reference to the response.

In regression with CO-type predictors, the total number of unique POs is massive, while only a limited number of them are sparsely observed within each replicate. It is advantageous to form groups of POs that are spatially contiguous, such that meaningful analysis can be conducted at a lower level of resolution. In many other applications, predictors are highly correlated, or collectively associated with the response, or domain knowledge exists suggesting the functional similarity among a group of variables. This has motivated a line of research on supervised clustering of predictors in forward regression settings. Examples include Hastie et al. (2001); Jörnsten and Yu (2003) and Dettling and Bühlmann (2004). The averaging operator on the predictors often leads to lower variance (Park et al., 2006).

Regularization methods such as elastic net (Zou and Hastie, 2005) or OSCAR (Bondell and Reich, 2008) can mitigate the multicollinearity issue and encourage grouping effects. Along this thread, Wang and Zhao (2017) recently proposed two tree-guide fused lasso (TFL) penalties, which effectively encode the topology of a phylogenetic tree in determining the taxonomic levels of microbes associated with a given phenotype. However, this approach does not model the variability in the predictors, while we model the conditional distributions of the predictors given the response through inverse regression, with possibilities of alleviating the effects of collinearity (Cook and Li, 2009). Moreover, Lasso-based penalties tend to over-shrink signals not close to zero (Armagan et al., 2011). We introduce a new multiscale prior that induces a locally adaptive shrinkage rule on each scale. This prior is used within our proposed spinlets method for supervised dimension reduction for SPIN predictors.

In Section 2, we introduce the data structure and notations. In Section 3, we describe our model-based SDR framework. Section 4 presents a tree-structured PX scheme and our induced multiscale shrinkage prior. A variational expectation-maximization (EM) algorithm for estimation is outlined in Section 5. In Section 6, we evaluate the performance of our approach with simulated data and demonstrate the practical utility through applications to
soccer analytics. The implementation of spinlets will be made available on Github.

2 Data Structure and Notations

2.1 Hierarchical Organization of Primitive Objects

To concisely represent the proximity information of POs (e.g., soccer passes), we define a tree structure in three steps: (i) choose the Euclidean distance metric between pairs of POs and compute a $Q \times Q$ distance matrix, $Q = \sum q_i$; (ii) construct a sparse similarity graph of POs $G$ by considering $K$ nearest neighbors; (iii) build a partition tree $T_h$ via recursively applying the METIS partitioning algorithm (Karypis and Kumar, 1998) on $G$. We construct a full binary tree via recursive METIS (rMETIS). In each step, a set of POs is split into two disjoint subsets. Figure 3 illustrates a sub-branch of $T_{10}$ with all assigned POs in the 16 groups plotted.

Figure 3: A sub-branch of the partition tree with 16 leave nodes (indicated by solid dots) produced by the rMETIS algorithm. Every internal node (indicated by hollow dots) on the coarse scale is connected with two child nodes on the finer scale.
2.2 Notations

The internal nodes in $T_h$ are indexed by $\mathcal{I}_{h-1} := \{(s, \ell) : 0 \leq s \leq h - 1, 1 \leq \ell \leq 2^s\}$, in which each parent node $(s, \ell)$ has two child nodes $(s + 1, 2\ell - 2 + t)$, where $t \in \{1, 2\}$. We denote by $\mathcal{C}_{s,\ell}$ the set of child nodes of $(s, \ell)$ and the set $\mathcal{F}_{s,\ell}$ all the nodes on the sub-branch rooted from node $(s, \ell)$. The tree $T_h$ is originated from the root node $(0, 1)$ with leaf nodes indexed by $L := \{(h, \ell) : 1 \leq \ell \leq 2^h\}$, $\mathcal{F}_{0,1} = \mathcal{I}_{h-1} \cup \mathcal{L}$. We define the partition induced by $L$ as the primary partition $\Pi_0 & L(T_h)$, which partitions $P$ into $m = 2^h$ groups on the finest scale and yields a primary vectorial representation $X \in \mathbb{Z}^m$ of COs, aligned across replicates. Our main goal is to determine a reductive rule $R(X)$ by pruning the tree $T_h$, such that the resulting representation retains the relevance to the response variable $Y$.

3 Tree-Guided Supervised Dimension Reduction

The above representation has not taken into account any information from the response. Hence, we further refine it along $T_h$ in a supervised manner.

3.1 Poisson Inverse Regression Model

According to Cook (2007), a sufficient reduction of the random vector $X$, denoted as $R(X)$, satisfies one of the three equivalent statements: (i) $X|Y, R(X)) \sim X|R(X);$ (ii) $Y|X \sim Y|R(X);$ (iii) $X \perp Y|R(X)$, where $\sim$ indicates equivalence in distribution and $\perp$ denotes independence. For replicate $i$ with response variable $Y_i$, we attach a random variable $X_{i,j} \in \mathbb{Z}$ to each leaf node $j$, counting the number of POs appearing in CO $E_i$ that fall in the leaf group $\Pi_j$. In order to explicitly model the variabilities in occurrences, we adopt an inverse regression formulation. This approach is largely motivated by poor performance we observed in implementing usual regression due to extreme multicollinearity issues. Sufficiency is guaranteed within our proposed Poisson inverse regression (PIR) model for $X_{i,j}$ conditionally on $Y_i$, $i = 1, \ldots, n$, $j = 1, \ldots, m$,

$$
(X_{i,j}|Y_i = y_i) \sim \text{Poisson}(\lambda_{i,j}), \quad \eta_{i,j}(y_i) = \ln(\lambda_{i,j}) = \alpha_j + \mu_i + y_i\beta_j, \quad (1)
$$

where $\alpha_j$ is the intercept for predictor $j$, $\mu_i$ is the baseline effect for replicate $i$, and $\beta_j$ is the regression coefficient for predictor $j$. The linear sufficient reduction $R_\beta(X)$ parameterized by $\beta$ is derived as follows (the replicate index $i$ is omitted for clarity).

**Proposition 1.** Letting $R_\beta(X) = \beta^T X$, under the inverse Poisson regression model (1), the distribution of $Y|X$ is the same as the distribution of $Y|R_\beta(X)$ for all values of $X$. 


Cook (2007) proves the sufficiency of $R_{\beta}(X) = \beta^T X$ for one-parameter exponential family models. Within this family, the PIR model (1) can be written in the following form,

$$f_j(x_j|Y = y) = a_j(\eta_j(y))b_j(x_j)\exp(x_j\eta_j(y)),\quad a_j(\eta_j(y)) = \exp[-\exp(\eta_j(y))], \quad b_j(x_j) = 1/x_j!$$

Accordingly, the joint probability mass function $f(x|y)$ of $X|(Y = y)$ can be written as

$$f(x|y) = g(\beta^T x, y)h(x),$$

where $g(\beta^T x, y) = \exp(y\beta^T x)\prod_{j=1}^{m} a_j(\eta_j(y))$ and $h(x) = \prod_{j=1}^{m} [b_j(x_j)\exp(x_j\alpha_j)]$. Thus, the sufficiency of reduction holds according to the Fisher-Neyman factorization theorem for sufficient statistics (Bickel and Doksum, 2015, Theorem 1.5.1, p. 43). The PIR model has a close connection with the multinomial inverse regression (MNIR) model (Taddy, 2013), though, the vector Poisson likelihood departs from multinomial likelihood by accounting for the variability of total number of POs in each replicate.

### 3.2 Reductive Operators: Deletion and Fusion

One reductive operator enabled by the $\beta$ parameterization from the PIR model (1) is the deletion of irrelevant leaf groups. One can see that $\beta_j = 0$ implies that $f(x_j|Y = y) \equiv f(x_j)$, that is, the number of POs in the leaf group $\Pi_j$ is independent of the value of $Y$. Another reductive operator on the tree is fusion. We observe that if $\beta_j = \beta_j' \neq 0$, $\forall j, j' \in D$, then $R_{\beta}(x)$ is a function depending on the predictors only through $\sum_{j \in D} X_j$, which is the total number of POs falling into the set $D$. Therefore, the practitioner can construct a lower resolution vectorial representation by merging the involved leaf sets into one set $D$ without loss of relevant information. The relevant signals are then captured on coarser scales. To ensure spatial contiguity, we require all leaves contained in $D$ to share at least one common ancestor node.

The grouping of highly correlated predictors in high-dimensional regression can be incorporated via fusion penalties (Tibshirani et al., 2005; Bondell and Reich, 2008), which encourage sparsity in the differences of coefficients. There exist several generalized fusion schemes that can take into account graph structure (She, 2010; Tibshirani and Taylor, 2011). However, these methods do not support multiscale nested grouping of predictors in accordance with the tree structure. For example, applying the pairwise fused lasso (She, 2010) to all pairs of variables tends to incorrectly encourage merging all the variables together with equal strengths. The TFL penalties (Wang and Zhao, 2017) require careful tuning of the regularization parameters across multiple scales.
4 Multiscale Shrinkage with Parameter Expansion

Parameter expansion (PX) (Liu et al., 1998) has been found useful not only for accelerating computations (Liu and Wu, 1999), but also for inducing new families of prior distributions (Gelman, 2004). In this section, we propose a new tree-structured PX scheme, which induces a multiscale shrinkage prior.

4.1 Tree Structured Parameter Expansion

For $j = 1, \ldots, m$, we denote by $A_j$ the “vertical” root-to-leaf path set in the tree $T_h$ connected to the leaf group $\Pi_j$, $j = 1, \ldots, m$. The path set $A_j$ includes all the nodes that it visits from the root node to the leaf node $j$. Meanwhile, we denote the “horizontal” descendant set $D_{s,\ell}$ as the set of leaf nodes who share a most recent common ancestor $(s, \ell), (s, \ell) \in I_{h-1}$, and specifically for $s = h$, we set $D_{h,j} \equiv L_j$, for $j = 1, \ldots, m$, for ease of notation. Figure 4 illustrates an example of a path set $A_8$ and an example of a descendant set $D_{2,4}$ with the common ancestor node $(2, 4)$.

![Figure 4: Illustration of $T_4$ with 16 leaf groups (solid dots). The green shaded region denotes a path set $A_8$ from root node $(0, 1)$ to leaf node $(4, 8)$, through three intermediate nodes: $(1, 1), (2, 2), (3, 4)$. The descendant set $D_{2,4}$ contains 4 leaf nodes (located in the dashed circle) with a most recent common ancestor $(2, 4)$ (indicated by the red octagon).](image)

There exists a dual relationship between random variables and coefficients based on these two notations. We can attach a random variable $Z_{i,s,\ell} \in \mathbb{Z}$ to each node $(s, \ell)$, where $Z_{i,s,\ell} = N(\mathcal{E}_i \cap D_{s,\ell})$ counts the appearances of POs in descendant set $D_{s,\ell}$ and...
\[
Z_{i,s,\ell} = \sum_{j \in D_{s,\ell}} X_{i,j}. \text{ Letting } \gamma_v \text{ be the coefficient for node } v \text{ visited by the path } A_j, \text{ we have } \beta_j = \sum_{v \in A_j} \gamma_v. \text{ Therefore, the sufficient reduction score } R_\beta(x_i) \text{ introduced in Section 3 can be re-expressed under the parameterization } \gamma \text{ on the partition tree } T_h, \]
\[
R_\beta(x_i) = \beta^T x_i = \sum_{j=1}^{m} x_{i,j} \beta_j = \sum_{j=1}^{m} \sum_{v \in A_j} \gamma_v = \sum_{s=0}^{h} \sum_{\ell=1}^{2^s} z_{i,s,\ell} \gamma_{s,\ell} = \gamma^T z_i = R_\gamma(x_i). \]

Clearly, \( R_\gamma(x_i) \) is also a linear sufficient reduction. The reparameterization changes neither the data likelihood of the PIR model (1), nor the sufficient reduction score.

### 4.2 Fused Generalized Double Pareto Prior

In Section 3.2, we introduced two reductive operations: deletion (if \( \beta_j = 0 \)) and fusion (if \( \beta_j = \beta_{j'}, \forall j, j' \in D_{s,\ell} \)) on the leaf partitions along the tree. However, exhaustive search for all possible schemes is prohibitive. Even for a binary tree \( T_3 \), these two operations in combination result in \( 458,330 \) different schemes. Alternatively, effective execution of the following two operations can be induced by regularization in the \( \gamma \) parameterization:

(i) **Deletion:** if \( \gamma_v = 0, \forall v \in A_j \), then \( \beta_j = \sum_{v \in A_j} \gamma_v = 0 \), which implies that the contributions of leaf predictor \( j \) across all the scales are pruned out.

(ii) **Fusion:** If \( \forall (s', \ell) \in F_{s,\ell}, \) their child nodes satisfy \( \gamma_{s'+1,2\ell-1} = \gamma_{s'+1,2\ell}, \) then \( \beta_j = \beta_{j'}, \forall j, j' \in D_{s,\ell} \), the leaf variables within \( D_{s,\ell} \) can be condensed into one variable.

Note that the \( \gamma \) parameterization is redundant; both conditions above are sufficient but not necessary. Based on the above observations, we impose generalized double Pareto (GDP) priors (Armagan et al., 2013) on \( \gamma \) and the pairwise differences between sibling nodes,

\[
\gamma_{s,\ell} \sim GDP(\xi_1, \alpha_1), \quad \gamma_{s',1,2\ell-1} - \gamma_{s'+1,2\ell} \sim GDP(\xi_2, \alpha_2), \quad (2)
\]

where \((s'+1,2\ell-1), (s'+1,2\ell) \in C_{s',\ell}, (s', \ell) \in I_{h-1} \) and \((s, \ell) \in F_0,1\). The first prior encourages sparsity on the individual coefficients and the second prior promotes sparsity on the differences between pairs of siblings with a common parent node \((s', \ell)\). These priors lead to a generalized fused lasso-type penalty (She, 2010; Tibshirani and Taylor, 2011), but the GDP prior corresponds to a reweighted \( \ell_1 \) penalty instead of \( \ell_1 \) (as will be seen in (5)), which better approximates the \( \ell_0 \)-like criterion (Candes et al., 2008).

For \( T_h \), the number of expanded parameters in \( \gamma \) is \( L = 2^{h+1} - 1 \). A natural question is whether there exists a multivariate prior on \( \gamma \) that could justify the compatibility of these
two GDP priors. To see this, we use the latent variable representation of the GDP prior introduced in Armagan et al. (2013). The first level of the hierarchy is written as,

$$\gamma_s, \ell \sim \mathcal{N}(0, \tau, \ell), \quad \gamma_{s'+1,2\ell-1} - \gamma_{s'+1,2\ell} \sim \mathcal{N}(0, \phi_{s'+1,2\ell-1,2\ell}).$$  \hfill (3)

We postulate a multivariate normal prior for the $L$-dimensional vector $\gamma \sim \mathcal{N}(0, \Lambda^{-1})$ with $L \times L$ precision matrix $\Lambda$, whose log marginal density is different than that of priors in (3) only up to a constant. The entries in $\Lambda$ as a function of $(\tau, \phi)$ can be found by square completing. It takes a block-diagonal form as follows,

$$\Lambda(\tau, \phi) = \text{blockdiag}[1/\tau_0, 1; \Omega_{0,1}; \Omega_{1,1}; \Omega_{1,2}; \ldots; \Omega_{h-1,1}, \ldots, \Omega_{h-1,m/2}],$$ \hfill (4)

where

$$\Omega_{s', \ell} = \begin{bmatrix} 1 & 0 \\ \tau_{s'+1,2\ell-1} & 1/\phi_{s'+1,2\ell-1,\ell} \end{bmatrix} + \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}, \quad \ell \in \mathcal{I}_{h-1}.$$

To complete the hierarchy of the multivariate GDP prior with $\gamma \sim \mathcal{N}(0, [\Lambda(\tau, \phi)]^{-1})$, we put $\tau_s, \ell \sim \text{Exp}(\lambda_s^2/2)$, $\lambda_s, \ell \sim \text{Ga}(\alpha_1, \eta_1)$, $(s, \ell) \in \mathcal{F}_{0,1}$, and $\phi_{s'+1,2\ell-1,2\ell} \sim \text{Exp}(\nu_{s'+1,2\ell-1,2\ell}^2/2)$, $\nu_{s'+1,2\ell-1,2\ell} \sim \text{Ga}(\alpha_2, \eta_2)$, $(s', \ell) \in \mathcal{I}_{h-1}$. So now we have a fused generalized double Pareto (fGDP) prior, which promotes the desired form of structured sparsity in $\gamma$, and enjoys a latent variable representation that makes the parameter estimation straightforward. Integrating out the latent variables $\Psi$, we obtain the marginal density of the fGDP prior, denoted by $\text{fGDP}(\gamma; T_h, \alpha_1, \eta_1, \alpha_2, \eta_2)$, whose logarithm takes the following form,

$$\ln p(\gamma) = \sum_{(s, \ell) \in \mathcal{F}_{0,1}} \left[ -\ln (2\xi_1) - (\alpha_1 + 1) \ln \left( 1 + \frac{|\gamma_{s, \ell}|}{\alpha_1 \xi_1} \right) \right]$$

$$+ \sum_{(s', \ell) \in \mathcal{I}_{h-1}} \left[ -\ln (2\xi_2) - (\alpha_2 + 1) \ln \left( 1 + \frac{|\gamma_{s'+1,2\ell-1} - \gamma_{s'+1,2\ell}|}{\alpha_2 \xi_2} \right) \right],$$ \hfill (5)

where $\xi_1 = \eta_1/\alpha_1$, $\xi_2 = \eta_2/\alpha_2$.

### 4.3 Multiscale Shrinkage in the Original Parameter Space

The tree-structured PX scheme introduced in Section 4.1 offers us a reparameterization: $\beta_j = \sum_{v \in A_j} \gamma_v$, $j = 1, \ldots, m$, which can be represented in matrix form as $\beta = D \gamma$, where $D$ is a $m \times L$ design matrix with binary entries, $m < L$. Each column in $D$ can be interpreted
as a basis function that encodes the piecewise smoothness at a different location and scale. For example, assuming \( h = 3 \), the number of leaves \( m = 2^3 = 8, \ L = 15 \), we have

\[
D = \begin{bmatrix}
1 & 1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\
1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
1 & 0 & 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 \\
1 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 \\
1 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\
\end{bmatrix}.
\]

Importantly, through PX, we have transformed the problem of multiscale shrinkage on the regression coefficients \( \beta \) across multiple scales on \( T_h \) into a structured shrinkage problem on the expanded parameters \( \gamma \), which can be conveniently addressed via the proposed fGDP prior. The hierarchical-Bayes representation of the multiscale shrinkage prior on \( \beta \) can be obtained via integrating out \( \gamma \). We have the conditional prior \( \beta | \tau, \phi \sim \mathcal{N}(0, D\Lambda(\tau, \phi)^{-1}D^T) \) and the priors on the latent variables \( \Psi := \{ \tau, \phi, \lambda, \nu \} \) do not change. However, the precision matrix \( D\Lambda(\tau, \phi)^{-1}D^T \) no longer exhibits a sparse block-diagonal structure as in (4), and the resulting EM procedure involves intractable expectations.

### 4.4 Incorporating Random Effects

We further assume each replicate is collected within a time window of length \( t_i, i = 1, \ldots, n \). To accommodate potential overdispersion and dependencies, we incorporate random effects in the model. The vector Poisson log-linear mixed regression model is written as follows,

\[
x_{i,j} \sim \text{Poisson}(\mu_{i,j}), \hspace{1cm} \mu_{i,j} = t_i e^{\eta_{i,j}}, \hspace{1cm} \eta_{i,j} = a + b_i + c_j + y_i \beta_j,
\]

where \((\beta_1, \ldots, \beta_m)\) is the fixed effect slope parameter for the \textit{m simple Poisson mixed regression} model (Hall et al., 2011b). The fixed effects measure the common association between the predictors and response, while the random effects allow replicates or primary groups to have their own baseline rates. The total, column and row random effects are \( a, b, c \), respectively. Constraints are needed for the identifiability of row and column scores \( b_i \) and \( c_j \), so we use the corner constraint (Yee and Hastie, 2003) \( b_1 \equiv c_1 \equiv 0 \) in this article. Gaussian priors on \( a, b = [b_2, \ldots, b_n] \) and \( c = [c_2, \ldots, c_m] \) are specified as follows,

\[
a \sim \mathcal{N}(0, \omega_a), \hspace{1cm} b_i \sim \mathcal{N}(0, \omega_b), \hspace{1cm} c_j \sim \mathcal{N}(0, \omega_c), \hspace{1cm} i = 2, \ldots, n, \hspace{1cm} j = 2, \ldots, m,
\]
with unknown variance parameters \( \omega = [\omega_a, \omega_b, \omega_c] \). Since \( \beta_j = d_j^T \gamma \), we have \( \eta_{i,j} = a + b_i + c_j + y_i d_j^T \gamma \). Note that the sufficiency of \( R_\gamma(x_j) \) established in Section 3.1 still holds conditional on the random effect terms (Taddy, 2013). In the next section, we introduce a penalized likelihood estimator of \( \gamma \), under the conditional likelihood \( \ell(\gamma, \omega) := \ln p(X|y, \gamma, \omega) \) with the proposed fGDP prior \( \gamma \sim \text{fGDP}(\alpha_1, \eta_1, \alpha_2, \eta_2) \) guided by \( T_h \).

5 Parameter Estimation

The hierarchical-Bayes representation of the fGDP prior facilitates an iterative EM-type algorithm for penalized estimation with (5). We adopt the type-I estimation framework (Figueiredo, 2003), which treats \( \Psi \) as latent variables and \( \{\gamma, \omega\} \) as parameters to optimize. The conditional likelihood of the model in (6) involves a \((n + m - 1)\)-dimensional integral,

\[
\ln p(X|y, \gamma, \omega) = \ln \int p(X|y, \gamma, a, b, c)p(a|\omega_a)p(b|\omega_b)p(c|\omega_c)da\,db\,dc,
\]

which is nonanalytic. Alternatively, we take a Gaussian variational approximation (GVA) of the posteriors of random effect variables \( U := \{a, b, c\} \), which provides a lower bound \( \ell(\gamma, \omega, \zeta, \kappa) \) of \( \ell(\gamma, \omega) \). Statistical properties of GVA for generalized linear mixed models are studied in Hall et al. (2011a,b) and Ormerod and Wand (2012), from a likelihood-based perspective. The resulting GVA estimator differs from the MLE but is asymptotically valid.

In our setting, the alternating steps are guaranteed to increase the following objective function (Neal and Hinton, 1998),

\[
\mathcal{F}(q, \gamma, \omega) = \langle \log P(X; \gamma, \Psi, U|y, \omega) \rangle_{q(\Psi, U)} + H[q(\Psi, U)],
\]

where \( q(\Psi, U) = q(\Psi)q(\zeta, \kappa(U)) \) naturally decouples into a factorized form, in which \( q(\Psi) \) is left in free-form and \( q(\zeta, \kappa) \) is parameterized as Gaussian with diagonal covariance. With \( t \) indexing the iterations, the overall algorithm contains the following alternating steps:

- **E-step:** Optimize \( \mathcal{F}(q, \gamma, \omega) \) w.r.t. the distribution of latent variables \( q(\Psi) \)

\[
q^{(t)}(\Psi) := \arg \max_{q(\Psi)} \mathcal{F}(q(\Psi), q^{(t-1)}(U), \gamma^{(t-1)}, \omega^{(t-1)}).
\]

- **Variational E-step:** Update the Gaussian variational parameters \( \{\zeta, \kappa\} \) such that

\[
\mathcal{F}(q^{(t)}(\Psi), q^{(t)}(U), \gamma^{(t-1)}, \omega^{(t-1)}) \geq \mathcal{F}(q^{(t)}(\Psi), q^{(t-1)}(U), \gamma^{(t-1)}, \omega^{(t-1)}).
\]
• **M-step.** Update the model parameters \( \{\gamma, \omega\} \) such that

\[
\mathcal{F}(q^{(t)}(\Psi), q^{(t)}(U), \gamma^{(t)}, \omega^{(t)}) \geq \mathcal{F}(q^{(t)}(\Psi), q^{(t)}(U), \gamma^{(t-1)}, \omega^{(t-1)}).
\]

In this algorithm, the variational parameters \( \{\zeta, \kappa\} \) and the model parameters \( \{\gamma, \omega\} \) are updated with gradient updates instead of exact maximization (Lange, 1995a,b). Therefore, it is a generalized EM algorithm (Dempster et al., 1977; Neal and Hinton, 1998), as both the E-step and M-step are taken partially. Note that the latent variables \( \Psi \) only appear in the prior, and the random effect terms \( U \) only appear in the likelihood,

\[
\mathcal{F}(q, \gamma, \omega) = \langle \ell_1(\Psi; \gamma) \rangle_{q(\Psi)} + \langle \ell_2(U; \gamma, \omega) \rangle_{q(U)},
\]

so we can discuss them separately.

### 5.1 Closed-Form Expectations in the Shrinkage Prior

We compute the expected value w.r.t \( \Psi \) in the complete log-posterior, given the current parameter estimates and the observed data. Note that the entropy term does not depend on \( (\gamma, \omega) \), so the relevant term in the E-step is

\[
\langle \ell_1(\Psi; \gamma) \rangle_{q(\Psi)} = \mathbb{E}_{p(\Psi|\gamma^{(t)}, \omega^{(t)}, x, y)}[\ell_1(\Psi, \gamma)],
\]

where

\[
\ell_1(\Psi, \gamma) = \sum_{(s, \ell) \in \mathcal{F}_{0,1}} \ln p(\gamma_{s, \ell}, \tau_{s, \ell}, \lambda_{s, \ell}|\alpha_1, \eta_1)
+ \sum_{(s', \ell') \in \mathcal{I}_{h-1}} \left[ \ln p(\delta_{s'+1,2\ell-1,2\ell}, \phi_{s'+1,2\ell-1,2\ell}, \nu_{s'+1,2\ell-1,2\ell}|\alpha_2, \eta_2) \right].
\]

According to the Gaussian scale mixture (GSM) representation of the GDP prior,

\[
\ln p(\gamma_{s, \ell}, \tau_{s, \ell}, \lambda_{s, \ell}|\alpha_1, \eta_1) = \ln p(\gamma_{s, \ell}|\tau_{s, \ell}) + \ln p(\tau_{s, \ell}|\lambda_{s, \ell}) + \ln p(\lambda_{s, \ell}|\alpha_1, \eta_1),
\]

and denoting the pairwise differences as \( \delta_{r,2\ell-1,2\ell} := \gamma_{r,2\ell-1} - \gamma_{r,2\ell}, r = 1, \ldots, h \), we have

\[
\ln p(\delta_{r,2\ell-1,2\ell}, \phi_{r,2\ell-1,2\ell}, \nu_{r,2\ell-1,2\ell}|\alpha_2, \eta_2) = \ln p(\delta_{r,2\ell-1,2\ell}|\phi_{r,2\ell-1,2\ell}) + \ln p(\phi_{r,2\ell-1,2\ell}|\nu_{r,2\ell-1,2\ell})
+ \ln p(\nu_{r,2\ell-1,2\ell}|\alpha_2, \eta_2).
\]

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Given the estimates from the previous iteration $\gamma^{(t)}$, the conditional posterior of latent variables $(\tau, \lambda)$ factorizes as

$$p(\tau, \lambda|\cdot) = \prod_{t \in T_{h-1} \cup \mathcal{L}} p(\tau_t, \lambda_t|\cdot), \quad p(\tau_t, \lambda_t|\cdot) = p(\tau_t|\lambda_t, -)p(\lambda_t|\cdot),$$

where $(\tau_t|\lambda_t, -) \sim \text{GIG}(p = 0.5, a = \lambda_t^2, b = \gamma_t^2)$. Integrating out $\tau_t$, we have $(\gamma_t|\lambda_t) \sim \text{DE}(\gamma_t; 0.1, /\lambda_t)$ and $(\lambda_t|\alpha_1, \eta_1) \sim \text{Ga}(\lambda_t; \alpha_1, \eta_1)$, so $(\lambda_t|\gamma_t, \alpha_1, \eta_1) \sim \text{Ga}(\alpha_1 + 1, |\gamma_t| + \eta_1)$, where $\text{DE}(x; \mu = 0, b) = \exp(-|x|/b)/2b$ refers to the Laplace distribution with scale parameter $b = 1/\lambda$ and $\text{GIG}(x; a, b, p)$ denotes the Generalized Inverse Gaussian (GIG) distribution, $\text{GIG}(x; a, b, p) = 0.5(a/b)^{p/2}x^{p-1}\exp(-ax + b/x)/K_p(\sqrt{ab})$, $(x > 0)$, and $K_p(\theta)$ is the modified Bessel function of the second kind.

Similarly, given the estimates of the $\delta^{(t)}$, the conditional posterior of latent variables $(\phi, \nu)$ also factorizes. Thus for every $(u, w) \in \mathcal{C}_s', \ell, (s', \ell) \in T_{h-1}$, we have $(\phi_{u,w}|\nu_{u,w}, -) \sim \text{GIG}(p = 0.5, a = \nu_u^2, b = \delta_{u,w}^2)$, and integrating out $\phi_{u,w}$, we have $(\delta_{u,w}|\nu_{u,w}) \sim \text{DE}(\delta_{u,w}; 0.1, /\nu_{u,w})$ and $(\nu_{u,w}|\alpha_2, \eta_2) \sim \text{Ga}(\nu_{u,w}; \alpha_2, \eta_2)$, so $(\nu_{u,w}|\delta_{u,w}, \alpha_2, \eta_2) \sim \text{Ga}(\alpha_2 + 1, |\delta_{u,w}| + \eta_2)$. Therefore,

$$\langle \ell_1(\Psi; \gamma) \rangle_{q(\Psi)} = \langle \ell_1(\Psi; \gamma) \rangle_{p(\Psi|\gamma^{(t)}, -)} = -\sum_{l=1}^L \frac{\gamma_l^2}{2} \langle \tau_l^{-1} \rangle - \sum_{(u,w) \in \mathcal{C}_s', \ell} \frac{\delta_{u,w}^2}{2} \langle \phi_{u,w}^{-1} \rangle. \quad (7)$$

We only need to find $\langle \tau_l^{-1} \rangle := \langle \rho_l \rangle$. According to the change of variable formula, $f(\rho_l) = \text{GIG}(\rho_l^{-1}; p, a, b)\rho_l^{-1} = \text{GIG}(\rho_l; -0.5, b, a) = \text{InvGau}(\rho_l; \sqrt{\lambda_l^2/\gamma_l^{2(t)}}, \lambda_l^2)$, we have

$$\mathbb{E}_{p(\rho_l|\lambda_l, -)}[\rho_l] = \lambda_l/|\gamma_l^{(t)}|,$$

$$\langle \rho_l \rangle = \mathbb{E}_{p(\lambda_l|\cdot)} \left[ \mathbb{E}_{p(\rho_l|\lambda_l, -)}[\rho_l] \right] = \frac{1}{|\gamma_l^{(t)}|} \mathbb{E}_{p(\lambda_l|\cdot)}[\lambda_l] = \frac{(\alpha_1 + 1)}{|\gamma_l^{(t)}|(|\gamma_l^{(t)}| + \eta_1)}, \quad (8)$$

and similarly denoting $\langle \phi_{u,w}^{-1} \rangle := \langle \nu_{u,w} \rangle$, we obtain

$$\langle \nu_{u,w} \rangle = \langle \phi_{u,w}^{-1} \rangle = \frac{(\alpha_2 + 1)}{|\delta_{u,w}^{(t)}|(|\delta_{u,w}^{(t)}| + \eta_2)}. \quad (9)$$

The GSM representation of the GDP priors determines a reweighting rule, as shown in (8) and (9), in which the weights depend only on the current estimate of the parameter $\gamma^{(t)}$ (or its differences), and the hyperparameters $(\alpha_1, \eta_1, \alpha_2, \eta_2)$.

The penalty terms in (7) can be organized in a quadratic form, where the block-diagonal matrix $\bar{\Lambda}$ can again be found by square completing,

$$\bar{\Lambda} = \text{blockdiag}[(\rho_{0,1}; \bar{\Omega}_{0,1}; \bar{\Omega}_{1,1}; \bar{\Omega}_{1,2}; \ldots; \bar{\Omega}_{h-1,1}, \ldots, \bar{\Omega}_{h-1,m/2}].$$
The log-priors for the random effect terms are
\[
\tilde{\Omega}_{s', \ell} = \begin{bmatrix}
\langle \rho_{s' + 1, 2\ell - 1} \rangle & 0 \\
0 & \langle v_{s' + 1, 2\ell - 1} \rangle
\end{bmatrix} + \begin{bmatrix}
1 & -1 \\
-1 & 1
\end{bmatrix}, \quad (s', \ell) \in \mathcal{I}_{h-1}.
\]

Therefore, \( \langle \ell_1(\Psi; \gamma) \rangle_{q(\Psi)} = \langle \ell_1(\Psi; \gamma) \rangle_{p(\gamma)} = -\gamma^T \Lambda \gamma / 2 \), which is the structured penalty that favors models with simpler structures conforming to \( \mathcal{T}_h \). The quadratic form is concave and differentiable, which makes gradient-based optimization methods suitable.

### 5.2 Gaussian Variational Approximation of the Likelihood

In our case, the log-likelihood for the Poisson mixed model in (6) is,
\[
\ln p(X | y, \gamma, a, b, c) = \sum_{i=1}^{n} \sum_{j=1}^{m} \left[ x_{i,j} \ln t_i - t_i \exp (\eta_{i,j}) - \ln (x_{i,j}) \right].
\]

The log-priors for the random effect terms are
\[
\ln p(a | \omega_a) = -\frac{1}{2} \ln (2\pi \omega_a) - \frac{a^2}{2\omega_a},
\]
\[
\ln p(b | \omega_b) = \sum_{i=2}^{n} \ln p(b_i | \omega_b) = -\frac{(n-1)}{2} \ln (2\pi \omega_b) - \sum_{i=2}^{n} \frac{b_i^2}{2\omega_b},
\]
\[
\ln p(c | \omega_c) = \sum_{j=2}^{m} \ln p(b_j | \omega_c) = -\frac{(m-1)}{2} \ln (2\pi \omega_c) - \sum_{j=2}^{m} \frac{c_j^2}{2\omega_c}.
\]

Let \( q(a) = \mathcal{N}(\zeta^a, \kappa^a) \), \( q(b_i) = \mathcal{N}(\zeta^b_i, \kappa^b_i) \), \( q(c_j) = \mathcal{N}(\zeta^c_j, \kappa^c_j) \), where \( \{\zeta^a, \zeta^b, \zeta^c\} \) are the mean parameters and \( \{\kappa^a, \kappa^b, \kappa^c\} \) are all positive parameters for the variances. Assuming the variational proposals are independent, the lower bound of \( \ln p(X | y, \gamma, \omega) \) is
\[
\ell(\gamma, \omega, \zeta, \kappa) = \mathbb{E}_q \left[ \sum_{i=1}^{n} \sum_{j=1}^{m} \ln p(x_{i,j} | y_i, a, b_i, c_j, \gamma) \right] + \mathbb{E}_{q(a)} \left[ \ln p(a | \omega_a) - \ln q(a) \right]
\]
\[
+ \sum_{i=2}^{n} \mathbb{E}_{q(b_i)} \left[ \ln p(b_i | \omega_b) - \ln q(b_i) \right] + \sum_{j=2}^{m} \mathbb{E}_{q(c_j)} \left[ \ln p(c_j | \omega_c) - \ln q(c_j) \right].
\]

\(^1\text{Note that for } b_1 \text{ and } c_1, \text{ we have fixed their value to } 0 \text{ therefore for notational convenience, we assume } \zeta^b_1 = \zeta^c_1 = 0 \text{ and } \kappa^b_1 = \kappa^c_1 = 0 \text{ in the likelihood term.}\)
Denoting \( \ell(\gamma, \omega, \zeta, \kappa) = \langle \ell_2(U; \gamma, \omega) \rangle_q(U) \), we have

\[
\langle \ell_2(U; \gamma, \omega) \rangle_q(U) = \sum_{i=1}^{n} \sum_{j=1}^{m} x_{i,j} \left( \zeta_i^a + \zeta_i^b + \zeta_i^c + y_i d_j^T \gamma \right) \\
- \sum_{i=1}^{n} \sum_{j=1}^{m} t_i \exp \left( \zeta_i^a + \zeta_i^b + \zeta_i^c + \frac{1}{2} (\kappa_i^a + \kappa_i^b + \kappa_i^c) \right) + y_i d_j^T \gamma \\
- \frac{1}{2\omega_a} \left( \zeta_i^a \right)^2 - \frac{1}{2\omega_b} \sum_{i=2}^{n} \left( \zeta_i^b \right)^2 - \frac{1}{2\omega_c} \sum_{j=2}^{m} \left( \zeta_j^c \right)^2 - \frac{1}{2} \ln(\omega_a) - \frac{n-1}{2} \ln(\omega_b) - \frac{m-1}{2} \ln(\omega_c) \\
+ \frac{1}{2} \left( \zeta_i^a \right)^2 + \frac{1}{2} \sum_{i=2}^{n} \left( \zeta_i^b \right)^2 + \frac{1}{2} \sum_{j=2}^{m} \left( \zeta_j^c \right)^2 + \frac{n+m-1}{2}.
\]

So in the variational E-step and the M-step, we update the variational parameters \( \{\zeta, \kappa\} \) and the model parameters \( \gamma \) through a quasi-Newton method with objective function

\[ Q(\gamma, \omega, \zeta, \kappa) := \ell(\gamma, \omega, \zeta, \kappa) - \gamma^T \tilde{\Lambda} \gamma / 2, \]

which only requires us to specify the first-order gradients (detailed in Appendix A).

In each M-step, we can also choose to optimize the prior parameter \( \omega \) via a fixed-point update. Setting the gradients \( D_{\omega_a} Q = D_{\omega_b} Q = D_{\omega_c} Q = 0 \), we obtain,

\[
\omega_a = \left( \zeta_i^a \right)^2, \quad \omega_b = \frac{1}{n-1} \sum_{i=1}^{n} \left( \zeta_i^b \right)^2, \quad \omega_c = \frac{1}{m-1} \sum_{j=1}^{m} \left( \zeta_j^c \right)^2.
\]

As suggested in Armagan et al. (2013), the hyper-parameters \( \{\alpha_1, \eta_1, \alpha_2, \eta_2\} \) can be either fixed or pre-learned from an initial Bayesian analysis based on griddy Gibbs sampling (Ritter and Tanner, 1992).

### 5.3 Computational Complexity

Our spinlets method is scalable to handle millions of POs. First, the \( Q \times Q \) distance matrix is constructed approximately by the k-d tree nearest neighbor search, which has \( O(Q) \) worst case complexity. Second, the rMETIS algorithm assigns the POs into \( m \) primary groups. After \( h \) phases, the set of POs \( \mathcal{P} \) is partitioned into \( m = 2^h \) leaf groups on \( \mathcal{T}_h \). The complexity of the bisection algorithm is \( O(|E| \log m) \), where \( |E| \) is the number of edges in
the similarity graph. Third, in balancing the per-iteration cost with the convergence rate in the variational EM algorithm, we adopt a quasi-Newton method with the L-BFGS algorithm (Liu and Nocedal, 1989), which uses a predetermined $c_0 = 100$ number of previous steps to form a low-rank Hessian approximation with complexity $O(m^2 c_0)$. As will be illustrated in Figure 6, the variational EM algorithm converges very fast in practice.

We measure the CPU time of these procedures on a standard laptop computer (Macbook Air, 1.6 GHz Intel Core i5, 8 GB 1600 MHz DDR3, Intel HD Graphics 6000 1536 MB). For $Q = 49,988$, constructing the nearest neighbor set (with $K = 1,500$ nearest neighbors) requires 15.97 seconds, computing the similarity matrix costs 68.58 seconds, and running the rMETIS algorithm (with tree depth $h = 9$) takes 52.87 seconds. Each iteration of the variational EM algorithm takes about 14.91 seconds to run.

6 Applications

In this section, we first compare the performance of various penalties within the GDP and fGDP families in a number of simulated examples (Section 6.1), and then use spinlets as an exploratory tool for visualizing spatial interaction networks from the FIFA World Cup 2018 dataset, while using the supervised information of interest (Section 6.2).

6.1 Simulation Study

We generate $n = \{25, 50, 100, 200\}$ observations from the model $x_{i,j} \sim \text{Poisson}(\mu_{i,j})$, $\mu_{i,j} = t_i e^{\eta_{i,j}}$, $\eta_{i,j} = a + b_i + c_j + y_i \beta_{j}^{*}$, $t_i \sim \text{Ga}(2, 1)$, $y_i \sim \text{Poisson}(0.5)$, for $i = 1, \ldots, n$, $j = 1, \ldots, m$, and $a \sim \mathcal{N}(0, 0.1)$, $b_{i'} \sim \mathcal{N}(0, 0.1)$, $c_{j'} \sim \mathcal{N}(0, 0.1)$, for $i' = 2, \ldots, n$, $j' = 2, \ldots, m$, $m = 2^h$, $h = 5$. We assume $\beta^*$ to be signals with multiscale structures in the following configurations:

(a) $\beta^* = (1, 1, 0, 0, 1, 1, 0, 1, 1, -1, -1, 0, 0, -1, -1, 0, 0, 0, -1, -1, 1, 1, 0, 0, 0, 0, 1, 1)$,

(b) $\beta^* = (1, \ldots, 1, 0, \ldots, 0, -1, \ldots, -1, 0, \ldots, 0, 1, \ldots, 1, -1, \ldots, -1, 0, \ldots, 0, 1, \ldots, 1)$,

(c) $\beta^* = (1, \ldots, 1, 0, \ldots, 0, -1, \ldots, -1, 0, \ldots, 0)$,

(d) $\beta^* = (1, 1, 0, 0, -1, \ldots, -1, 1, 0, \ldots, 0, 1, \ldots, 1)$. 

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6.1.1 Baseline Methods

Denoting the GDP prior as $\text{GDP}(\alpha, \eta)$, we consider the following baseline methods (detailed derivations provided in Appendix B) operating on the original parameter $\beta$:

1. **GDP-0**: no prior, $\beta_j \sim \text{GDP}(-1, 1)$, and $j = 1, \ldots, m$,

2. **GDP prior with default parameters**, $\beta_j \sim \text{GDP}(1, 1)$, and $j = 1, \ldots, m$,

3. **Fused lasso signal approximation (FLSA)** (Friedman et al., 2007) implemented with the GDP prior: $\beta_j \sim \text{GDP}(1, 1)$, $\beta_j' - \beta_{j+1}' \sim \text{GDP}(1, 1)$, and $j' = 1, \ldots, m - 1$,

4. **Pairwise fused lasso (PFL-S)** (Petry et al., 2011) with the deletion and fusion penalties weighted by 0.8 and 0.2 respectively, implemented with the GDP prior: $\beta_j \sim \text{GDP}(1, 1)$, and $\beta_j - \beta_k \sim \text{GDP}(1, 1)$, $j, k = 1, \ldots, m$, and $j \neq k$.

5. **Pairwise fused lasso (PFL-F)** (Petry et al., 2011) with the deletion and fusion penalties weighted by 0.2 and 0.8 respectively (implementation is similar as above).

We also consider the following structural regularizers on the expanded parameter $\gamma$. All of them are derived from the $f\text{GDP}(\alpha_1, \eta_1, \alpha_2, \eta_2)$ family:

6. **fGDP-S**: deletion only, $\gamma \sim f\text{GDP}(1, 1, -1, 1)$,

7. **fGDP-F**: fusion only, $\gamma \sim f\text{GDP}(-1, 1, 1, 1)$,

8. **fGDP**: with default parameters, $\gamma \sim f\text{GDP}(1, 1, 1, 1)$,

9. **fGDP-NJ**: with Normal-Jeffrey’s parameters, $\gamma \sim f\text{GDP}(0, 0, 0, 0)$.

To investigate the sensitivity to the hyperparameters $\{\alpha_1, \eta_1, \alpha_2, \eta_2\}$, we additionally include: (10) **fGDP1**: $\gamma \sim f\text{GDP}(1, 0.1, 1, 0.1)$, (11) **fGDP2**: $\gamma \sim f\text{GDP}(1, 0.01, 1, 0.01)$, (12) **fGDP3**: $\gamma \sim f\text{GDP}(1, 0.001, 1, 0.001)$, (13) **fGDP4**: $\gamma \sim f\text{GDP}(0.5, 0.01, 0.5, 0.01)$, (14) **fGDP5**: $\gamma \sim f\text{GDP}(2, 0.01, 2, 0.01)$, and (15) **fGDP6**: $\gamma \sim f\text{GDP}(5, 0.01, 5, 0.01)$. All these 15 methods share the same random initialization of parameters.
Figure 5: Boxplots of the F1 Scores and RMSE for 50 simulations. Configurations (a)∼(d) are shown on row 1 ∼ 4, respectively. The initial greek letter (β or γ) indicates the parameter space of the baseline methods.
6.1.2 Performance Evaluation

We perform 50 replications for every simulation scenario. To evaluate the performance, we use the F1 score = $2 \times (\text{precision} \times \text{recall}) / (\text{precision} + \text{recall})$ as a metric for reduction. In particular, for selection, we examine whether the non-zero regression coefficients in the $m$ leaf groups are detected. For fusion, we make $2^h - 1$ binary decisions on whether the regression coefficients within the descendant set $D_{s',\ell}$ are all equal, for every internal node $(s', \ell) \in \mathcal{I}_{h-1}$. We also provide the relative mean square error (RMSE) as a reference metric for signal recovery RMSE = $||\hat{\beta} - \beta^*||_F / ||\beta^*||_F$.

The results are illustrated in Figure 5. The results across rows demonstrate the adaptation ability of our PX-based fGDP approaches in recovering signals with multi-level and multiplex smoothness. In general, the performance improves with the replicate size. When replicate size is relatively small, regularization helps boost the performance. Methods encouraging fusion produce better results in terms of F1 score (fusion) than those only encouraging selection. Note that by encouraging the expanded parameters on the root-to-leaf path to be sparse, the fGDP-S method is also able to encourage fusion in an indirect way.

6.1.3 Hyperparameter Sensitivity

We observe that the default choice $\alpha = \eta = 1$ and the Normal-Jeffrey’s choice $\alpha = \eta = 0$ yield sub-optimal results. As the parameters in the PX space are redundant, a high level of shrinkage is required, demanding a small $\eta$ parameter. The PX-based fGDP approaches (fGDP1 ~ fGDP6) with $\eta \in (10^{-3}, 10^{-1})$ compare favorably to the other methods in terms of both F1 scores (fusion and selection) and RMSE. Due to the adaptive shrinkage mechanism, the $\alpha$ parameters are less sensitive, we observed that $\alpha \in (0.5, 5)$ works reasonably well. In the original parameter space, the only method standing out in terms of the F1 scores is the fusion-dominated pairwise fused lasso (PFL-F) approach; however, this approach suffers from the inaccurate prior knowledge discussed in Section 3.2. As a result, it yields the worst RMSE performance among all the baselines considered.

6.1.4 Convergence

We choose the convergence criteria to be $||\beta^{(t)} - \beta^{(t-1)}||_F < 10^{-6}$, and for the PX-based method, this is $||D\gamma^{(t)} - D\gamma^{(t-1)}||_F < 10^{-6}$. The quasi-Newton updates are performed with L-BFGS, with 1,000 the maximum number of iterations allowed. We use the MATLAB solver minFunc (Schmidt, 2005). Setting the maximum iterations of variational EM to be
50, the number of iterations until convergence is reported in Figure 6. As expected, the PX-based approaches converge much faster than the non-PX based approaches.

The PX-based approaches only converge to one of the many local optima. We repeated the fGDP2 approach with hyper-parameters $\alpha_1 = \alpha_2 = 1$, $\eta_1 = \eta_2 = 0.01$ with 500 different random initializations. For every pair of different runs $a, b \in \{1, \ldots, 500\}$ and $a \neq b$, we calculate the pairwise distances $||\hat{\beta}_a - \hat{\beta}_b||_F$ and $||\hat{\gamma}_a - \hat{\gamma}_b||_F$ as a metric for variability. The results under configuration (d) with $n = 200$ are summarized in Figure 7, which show that the algorithm converges to a large number of different local optimal solutions in the auxiliary space; however, when reducing to the original space, they all map to solutions with comparable quality lying within a close neighborhood around the ground truth $\beta^*$.  

6.2 Supervised Dimension Reduction of Soccer Passing Networks

As a team sport, soccer is characterized by its free-flowing nature (Gudmundsson and Horton, 2017). The spatial interaction networks provide a concise abstraction of the team play on the pitch, which capture the essence of soccer as an invasion-territorial sport. Our spinlets approach provides a useful tool for further reducing complexity, taking advantage of both the passing network structure and the response relevance. On the FIFA World Cup 2018 dataset, we consider two responses of interest in the two tasks below:
Figure 7: Simulation with different random initializations. Left panel: boxplots of pairwise distance between the estimated $\beta$ or $\gamma$ parameters across the 500 runs. Right panel: estimations of $\beta$ (cyan lines) comparing against the ground truth (black circled line).

1. **Task 1**: Team performance measured by the goal difference (i.e., goal scored minus goal conceded) in the 128 game plays (unique team-game pairs).

2. **Task 2**: The urgency and tiredness status of the game, indicated by whether the data are collected after 70 minutes. This division of game play into two phases results in $128 \times 2 = 256$ replicates with binary responses.

We compare three algorithms: (1) rMETIS with $h = 9$, (2) a single-scale selection-only (S3O) approach with the default GDP prior on $\beta$, and (3) Spinlets with the fGDP2 prior on $\gamma$. The threshold for the regression coefficients to be considered as (approximately) equal is set to be 0.005. The rMETIS algorithm provides a common starting point of CG representation for both S3O and Spinlets. Interestingly, the same game can be seen with different eyes, when the practitioner picks a different response variable. Figure 8 and 9 illustrate the reductive representations of exactly the same games with two different types of response. In task 1 we consider team performance measured by the goal differences, while in task 2 we consider whether the passing network is collected in a relatively late phase of the game, when the time is running out and the players are getting physically and mentally tired. Spinlets reveals a clear pattern that France surrenders possession, strikes back on the counter with long vertical passes, and plays directly towards forward players. In contrast, Croatia relies more on short and horizontal passes, especially in the first 70 minutes.

The magnitude of the estimated regression coefficients $\hat{\beta}$ indicates the strength of association with the response. With both both selection and fusion, Spinlets produces more concise representations than S3O and allows for non-uniform resolutions. Figure 10
Figure 8: SPIN representations of France in the World Cup Final 2018, under the supervision of goal difference (first row), or under the supervision of game phase indicator in the first 70 minutes (second row), and after 70 minutes (third row).
Figure 9: SPIN representations of Croatia in the World Cup Final 2018, under the supervision of goal difference (first row), or under the supervision of game phase indicator in the first 70 minutes (second row), and after 70 minutes (third row).
(b) suggests that the cross-passes from the two wings seem relatively inefficient in creating
goals, with the exception of a short pass around the left corner of the penalty area. In
contrast, Figure 10 (d) indicates that teams tend to control the midfield more in the first 70
minutes, while pushing for the goal by passing more in the opposing half after 70 minutes.

Figure 10: The estimated regression coefficients \( \hat{\beta} \) in the two tasks.

To illustrate the predictive power of the reductive representation, we plot the SDR score
versus the response in Figure 11. For the PIR mixed model, the sufficiency of the SDR score
holds conditionally on the replicate-specific random effects \([a, a + b]\), so we cut \([\zeta_a, \zeta_a + \zeta_b]\),
the estimated mean of random effects, into three intervals, and present the results in three
separate panels. Both S3O and Spinlets are regularized approaches, in which fitting the
data is not the only goal. Comparing to S3O, Spinlets produces more parsimonious results
with little or no sacrifice in discriminative power, as shown in Figure 11.
(a) Task 1 (goal difference): S3O

(b) Task 1 (goal difference): Spinlets

(c) Task 2 (game phase): S3O

(d) Task 2 (game phase): Spinlets

Figure 11: SDR score v.s. response in the two tasks, separated into 3 groups according to the estimated mean of the replicate-specific random effects.
7 Discussion

In this article, we have introduced spinlets—a supervised dimension reduction method for spatial interaction networks using information on the spatial locations of each pass and also a response variable in constructing a multiscale representation. Specifically, the dimension reduction is conducted via a top-down partitioning of the similarity graph and a bottom-up pruning of the partition tree. Instead of cutting at a single height of a given tree, we select multiple tree heights for different branches of the tree adaptively, which yields representations with mixed granularities. The regularization prevents the information preserved in the lower-dimensional representation from being dominated by the supervisory signal without enough conformity to the spatial network data structures. In addition, our approach can be interpreted as an empirical Bayes approach, which estimates a hierarchical tree organization of the data in a first stage.

Besides the sports application studied in this article, our spinlets approach can accommodate massive-scale network predictors or time series predictors with high sampling rate; both are pressing needs in neuroscience. Potentially further improvements on the flexibility and utility of spinlets are possible, such as zero-inflated variants, SDR with multiple responses and covariate adjustment.

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A Gradients in the M-Step

The vectors $\zeta$ and $\kappa$ are variational parameters and should be chosen to make $\mathcal{L}(\gamma, \omega, \zeta, \kappa)$ as close as possible to $\mathcal{L}(\gamma, \omega)$. Given $q(\Psi)$ and denoting $\mathcal{F}(q(\Psi), \gamma, \omega) = Q(\gamma, \omega, \zeta, \kappa)$, we have
• Gradients of $\boldsymbol{\gamma}$: Denoting the gradients of $Q(\boldsymbol{\gamma}, \omega, \zeta, \kappa)$ over $\gamma_l$ as $D_{\gamma_l}Q$, we have

$$D_{\gamma_l}Q = \sum_{i=1}^{n} \sum_{j=1}^{m} \epsilon_{i,j} y_i d_{j,l} - \tilde{A}_{i,j}(t) \gamma_l, \quad \epsilon_{i,j} = x_{i,j} - \bar{x}_{i,j},$$

where $\bar{x}_{i,j} = t_i \exp[\zeta^a + \zeta^b + \zeta^c + \frac{1}{2}(\kappa^a + \kappa^b + \kappa^c) + y_i \sum_{l=1}^{L} d_{j,l} \gamma_l]$.

• Gradients of $\boldsymbol{\zeta}$: Denoting the gradients of $Q(\boldsymbol{\gamma}, \omega, \zeta, \kappa)$ over $\zeta^a$, $\zeta^b$, and $\zeta^c$ as $D_{\zeta^a}Q$, $D_{\zeta^b}Q$, and $D_{\zeta^c}Q$ respectively, we have

$$D_{\zeta^a}Q = -\frac{\zeta^a}{\omega_a} + \sum_{i=1}^{n} \sum_{j=1}^{m} \epsilon_{i,j}, \quad D_{\zeta^b}Q = -\frac{\zeta^b}{\omega_b} + \sum_{j=1}^{m} \epsilon_{i,j}, \quad D_{\zeta^c}Q = -\frac{\zeta^c}{\omega_c} + \sum_{i=1}^{n} \epsilon_{i,j}.$$  

• Gradients of $\boldsymbol{k}$: To ensure positivity of the variance parameters $\kappa$, we apply the log reparameterization on $\kappa$. Denoting the gradients of $Q(\boldsymbol{\gamma}, \omega, \zeta, \kappa)$ over $k^a = \log(\kappa^a)$, $k^b = \log(\kappa^b)$, and $k^c = \log(\kappa^c)$ as $D_{k^a}Q$, $D_{k^b}Q$, and $D_{k^c}Q$ respectively, we have

$$D_{k^a}Q = -\frac{\exp(k^a)}{2\omega_a} + \frac{1}{2} - \frac{1}{2} \sum_{i=1}^{n} \sum_{j=1}^{m} \bar{x}_{i,j} \exp(k^a),$$

$$D_{k^b}Q = -\frac{\exp(k^b)}{2\omega_b} + \frac{1}{2} - \frac{1}{2} \sum_{j=1}^{m} \bar{x}_{i,j} \exp(k^b),$$

$$D_{k^c}Q = -\frac{\exp(k^c)}{2\omega_c} + \frac{1}{2} - \frac{1}{2} \sum_{i=1}^{n} \bar{x}_{i,j} \exp(k^c).$$

### B GDP Family Priors on $\boldsymbol{\beta}$

**The GDP Prior** The GDP penalty term is $\log p(\beta) = \sum_{j=1}^{m} \log p(\beta_j) = \sum_{j=1}^{m} - \log(2\xi) - (\alpha + 1) \log(1 + \frac{[\beta_j]}{\alpha \xi})$. In the E-Step, we have $\langle \beta_j \rangle = (\alpha + 1)/[|\beta_j|(|\beta_j| + \eta)]$. In the M-step, the gradient w.r.t $\beta_j$ can be written as,

$$D_{\beta_j}Q = \sum_{i=1}^{n} \epsilon_{i,j} y_i - \langle \beta_j \rangle \beta_j, \quad \epsilon_{i,j} = x_{i,j} - \bar{x}_{i,j},$$

where $\bar{x}_{i,j} := t_i \exp[\zeta^a + \zeta^b + \zeta^c + \frac{1}{2}(\kappa^a + \kappa^b + \kappa^c) + y_i \beta_j]$ and the gradients w.r.t other parameters do not change.
GDP-based FLSA  The GDP-based FLSA penalty term is

\[
\log p(\beta) = \sum_{j=1}^{m} \log p(\beta_j) = \sum_{j=1}^{m} \left[ -\log (2\xi_1) - (\alpha_1 + 1) \log \left( 1 + \frac{|\beta_j|}{\alpha_1 \xi_1} \right) \right] \\
+ \sum_{j'=1}^{m-1} \left[ -\log (2\xi_2) - (\alpha_2 + 1) \log \left( 1 + \frac{|\beta_{j'} - \beta_{j'+1}|}{\alpha_2 \xi_2} \right) \right].
\]

In the E-Step, we have

\[
\langle \rho_j \rangle = (\alpha_1 + 1)/[|\beta_j(t)|(|\beta_j(t)| + \eta_1)], \quad \langle \nu_j \rangle = (\alpha_2 + 1)/[|\delta_j(t)|(|\delta_j(t)| + \eta_2)],
\]

where \(\delta_j(t) = \beta_{j'}(t) - \beta_{j'+1}(t)\). In the M-step, the gradient w.r.t \(\beta_j\) can be written as

\[
D_{\beta_j} Q = \sum_{i=1}^{n} \epsilon_{i,j} y_i - \tilde{\Lambda}^{(t)} \beta,\text{ where}
\]

\[
\tilde{\Lambda}^{(t)} = \begin{bmatrix}
\langle \rho_1 \rangle + \langle \nu_1 \rangle, & -\langle \nu_1 \rangle, & \ldots, & -\langle \nu_1 \rangle, & -\langle \nu_2 \rangle, & \ldots, & -\langle \nu_2 \rangle, & \ldots, & -\langle \nu_m \rangle, & -\langle \nu_m \rangle
\\
-\langle \nu_1 \rangle, & \langle \rho_2 \rangle + \langle \nu_1 \rangle + \langle \nu_2 \rangle, & \ldots, & -\langle \nu_2 \rangle, & -\langle \nu_3 \rangle, & \ldots, & -\langle \nu_3 \rangle, & \ldots, & -\langle \nu_m \rangle, & -\langle \nu_m \rangle
\\
-\langle \nu_2 \rangle, & -\langle \nu_3 \rangle, & \ldots, & -\langle \nu_3 \rangle, & -\langle \nu_4 \rangle, & \ldots, & -\langle \nu_4 \rangle, & \ldots, & -\langle \nu_m \rangle, & -\langle \nu_m \rangle
\\
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots
\\
-\langle \nu_{m-1} \rangle, & -\langle \nu_m \rangle, & \ldots, & -\langle \nu_m \rangle, & -\langle \nu_{m+1} \rangle, & \ldots, & -\langle \nu_{m+1} \rangle, & \ldots, & -\langle \nu_{m+1} \rangle, & -\langle \nu_{m+1} \rangle
\\
-\langle \nu_{m-1} \rangle, & -\langle \nu_{m-1} \rangle, & \ldots, & -\langle \nu_{m-1} \rangle, & -\langle \nu_{m-1} \rangle, & \ldots, & -\langle \nu_{m-1} \rangle, & \ldots, & -\langle \nu_{m-1} \rangle, & -\langle \nu_{m-1} \rangle
\end{bmatrix}
\]

GDP-based PFL  The GDP-based PFL penalty term is

\[
\log p(\beta) = \sum_{j=1}^{m} \log p(\beta_j) = \theta \sum_{j=1}^{m} \left[ -\log (2\xi_1) - (\alpha_1 + 1) \log \left( 1 + \frac{|\beta_j|}{\alpha_1 \xi_1} \right) \right] \\
+ (1 - \theta) \sum_{j<k} \left[ -\log (2\xi_2) - (\alpha_2 + 1) \log \left( 1 + \frac{|\beta_j - \beta_k|}{\alpha_2 \xi_2} \right) \right],
\]

where \(\theta \in [0,1]\) is the weight parameter that balances selection with fusion. In the E-Step, we have

\[
\langle \rho_j \rangle = \theta(\alpha_1 + 1)/[|\beta_j(t)|(|\beta_j(t)| + \eta_1)], \quad \langle \nu_{j,k} \rangle = (1 - \theta)(\alpha_2 + 1)/[|\delta_{j,k}(t)|(|\delta_{j,k}(t)| + \eta_2)],
\]

where \(\delta_{j,k} = \beta_j(t) - \beta_{k}(t)\). Similarly, in the M-step the gradient w.r.t \(\beta_j\) can be written as

\[
D_{\beta_j} Q = \sum_{i=1}^{n} \epsilon_{i,j} y_i - \tilde{\Lambda}^{(t)} \beta,\text{ where}
\]

\[
\tilde{\Lambda}^{(t)} = \begin{bmatrix}
\langle \rho_1 \rangle + \sum_{k \neq 1} \langle \nu_{1,k} \rangle, & -\langle \nu_{1,k} \rangle, & \ldots, & -\langle \nu_{1,k} \rangle, & -\langle \nu_{1,2} \rangle, & \ldots, & -\langle \nu_{1,2} \rangle, & \ldots, & -\langle \nu_{1,m} \rangle, & -\langle \nu_{1,m} \rangle
\\
-\langle \nu_{1,2} \rangle, & \langle \rho_2 \rangle + \sum_{k \neq 2} \langle \nu_{2,k} \rangle, & \ldots, & -\langle \nu_{2,3} \rangle, & -\langle \nu_{2,3} \rangle, & \ldots, & -\langle \nu_{2,3} \rangle, & \ldots, & -\langle \nu_{2,m} \rangle, & -\langle \nu_{2,m} \rangle
\\
-\langle \nu_{1,m} \rangle, & -\langle \nu_{2,m} \rangle, & \ldots, & -\langle \nu_{2,m} \rangle, & -\langle \nu_{3,m} \rangle, & \ldots, & -\langle \nu_{3,m} \rangle, & \ldots, & -\langle \nu_{3,m} \rangle, & -\langle \nu_{3,m} \rangle
\\
\vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \ddots & \vdots & \vdots
\\
-\langle \nu_{m-1,m} \rangle, & -\langle \nu_{m-1,m} \rangle, & \ldots, & -\langle \nu_{m-1,m} \rangle, & -\langle \nu_{m-1,m} \rangle, & \ldots, & -\langle \nu_{m-1,m} \rangle, & \ldots, & -\langle \nu_{m-1,m} \rangle, & -\langle \nu_{m-1,m} \rangle
\\
-\langle \nu_{m-1,m} \rangle, & -\langle \nu_{m-1,m} \rangle, & \ldots, & -\langle \nu_{m-1,m} \rangle, & -\langle \nu_{m-1,m} \rangle, & \ldots, & -\langle \nu_{m-1,m} \rangle, & \ldots, & -\langle \nu_{m-1,m} \rangle, & -\langle \nu_{m-1,m} \rangle
\end{bmatrix}
\]
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