Bayesian nonparametric scalar-on-image regression via Potts-Gibbs random partition models

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Abstract

Scalar-on-image regression aims to investigate changes in a scalar response of interest based on high-dimensional imaging data. We propose a novel Bayesian nonparametric scalar-on-image regression model that utilizes the spatial coordinates of the voxels to group voxels with similar effects on the response to have a common coefficient. We employ the Potts-Gibbs random partition model as the prior for the random partition in which the partition process is spatially dependent, thereby encouraging groups representing spatially contiguous regions. In addition, Bayesian shrinkage priors are utilised to identify the covariates and regions that are most relevant for the prediction. The proposed model is illustrated using the simulated data sets.

Keywords Bayesian nonparametric · Gibbs-type priors · Potts model · Clustering · Generalised Swendsen-Wang · High-dimensional imaging data

1 Introduction

Through advances in data acquisition, vast amounts of high-dimensional imaging data are collected to study phenomena in many fields. Such data are common in biomedical studies to understand a disease or condition of interest Craddock et al. [2009], Fan et al. [2008], Shi et al. [2014], Van Walderveen et al. [1998], and in other fields such as psychology Davatzikos et al. [2005], Sun et al. [2009], social sciences Ferwerda et al. [2016], Hum et al. [2011], Kim and Kim [2018], Samany [2019], economics Henderson et al. [2009], Naik et al. [2016, 2017], climate sciences O’Neill [2013], O’Neill et al. [2013], environmental sciences Debois et al. [2015], Gundlach-Graham et al. [2015], Maloof et al. [2020] and more. While extracting features from the images based on predefined regions of interest favours interpretation and eases computational and statistical issues, changes may occur in only part of a region or span multiple structures. In order to capture the complex spatial pattern of changes and improve accuracy and understanding of the underlying phenomenon, sophisticated approaches are required that utilize the entire high-dimensional imaging data. However, the massive dimension of the images, which is often in the millions, combined with the relatively small sample size, which at best is usually in the hundreds, pose serious challenges.

In the statistical literature, this is framed as a scalar-on-image regression (SIR) problem Goldsmith et al. [2014], Huang et al. [2013], Kang et al. [2018], Li et al. [2015]. SIR belongs to the “large p, small n” paradigm; thus, many SIR models utilise shrinkage methods that additionally incorporate the spatial information in the image Goldsmith et al. [2014], Huang et al. [2013], Kang et al. [2018], Lee and Cao [2021], Li et al. [2015], Mehrotra and Maity [2021], Reiss et al. [2011], Smith and Fahrmeir [2007], Wang et al. [2017]. In the SIR problem, the covariates represent the image value at a single pixel/voxel, i.e. a very tiny region, and the effect on the response is most often weak, unreliable and difficult to interpret. Moreover, neighbouring pixels/voxels are highly correlated, making standard regression methods, even with shrinkage, problematic due to multicollinearity.

To overcome these difficulties, we develop a novel Bayesian nonparametric (BNP) SIR model that extracts interpretable and reliable features from the images by grouping voxels with similar effects on the response to have a common coefficient. Specifically, we employ the Potts-Gibbs model Li et al. [2020] as the prior of the random image partition to encourage spatially dependent clustering. In this case, features represent regions that are automatically defined to be the most discriminative. This not only improves the signal and eases interpretability, but also reduces the computational burden by drastically decreasing the image dimension and addressing the multicollinearity problem. Moreover, it allows sharp discontinuities in the coefficient image across regions, which may be relevant in medical applications to capture irregularities Wang et al. [2017].

In this direction, Li et al. [2015] proposed the Ising-DP SIR model, which combines an Ising prior to incorporate the spatial information in the sparsity structure with a Dirichlet Process (DP) prior to group coefficients. Still, the spatial information is only incorporated in the sparsity structure and not in the BNP clustering model, which could result
in regions that are dispersed throughout the image. Instead, we propose to incorporate the spatial information in the random partition model, encouraging spatially contiguous regions. Further advantages of the nonparametric model include a data-driven number of clusters, interpretable parameters, and efficient computations. Moreover, we combine this with heavy-tailed shrinkage priors [Song and Liang 2017] to identify relevant covariates and regions.

The remainder of this article is organized as follows. Section 2 outlines the development of the SIR model based on the Potts-Gibbs models. Section 3 derives the MCMC algorithm for posterior inference using the generalized Swendsen-Wang (GSW) [Xu et al. 2016] algorithm for efficient split-merge moves that take advantage of the spatial structure. Section 4 illustrates the methods through simulation studies. Section 5 concludes with a summary and future work.

2 Model Specification

We introduce the statistical models that form the basis of the proposed Potts-Gibbs SIR model: SIR, random image partition model and shrinkage prior.

2.1 Scalar-on-Image Regression

SIR is a statistical linear method used to study and analyse the relationship between a scalar outcome and two or three-dimensional predictor images under a single regression model [Goldsmith et al. 2014, Huang et al. 2013, Kang et al. 2018, Li et al. 2015]. For each data point, \( i = 1, \ldots, n \), we have

\[
y_i = w_i^T \beta + x_i^T \beta + \epsilon_i, \quad \epsilon_i \sim N(0, \sigma^2),
\]

where \( y_i \) is a scalar continuous outcome measure, \( w_i = (w_{i1}, \ldots, w_{iq})^T \in \mathbb{R}^q \) is a \( q \)-dimensional vector of covariates, and \( x_i = (x_{i1}, \ldots, x_{ip})^T \in \mathbb{R}^p \) is a \( p \)-dimensional image predictor. Each \( x_{ij} \) indicates the value of the image at a single pixel with spatial location \( s_j = (s_{j1}, s_{j2})^T \in \mathbb{R}^2 \) for \( j = 1, \ldots, p \). We define \( \beta = (\beta_1, \ldots, \beta_p)^T \in \mathbb{R}^p \) as a \( q \)-dimensional fixed effects vector and \( \beta = (\beta(s_1), \ldots, \beta(s_p)) \) as the spatially varying coefficient image described on the same lattice as \( x_i \). We model the high-dimensional \( \beta \) by spatially clustering the pixels into \( M \) regions and assuming common coefficients \( \beta_1^*, \ldots, \beta_M^* \) within each cluster, i.e. \( \beta_j = \beta_j^* \) given the cluster label \( z_j = m \). Thus, the prior on the coefficient image is decomposed into two parts: the random image partition model for spatially clustering the pixels and a shrinkage prior for the cluster-specific coefficients \( \beta^* = (\beta_1^*, \ldots, \beta_M^*)^T \).

The SIR model in (1) can be extended for other types of responses through a generalized linear model framework (GLM) [McCullagh and Nelder 1999].

2.2 Random Image Partition Model

The image predictors are observed on a spatially structured coordinate system. Exchangeability is indeed no longer the proper assumption as the images contain covariate information, that we wish to leverage to improve model performance in this high-dimensional setting. To do so, we combine BNP random partition models, which avoid the need to prespecify the number of clusters, allowing it be determined and grow with the data, with a Potts-like spatial smoothness component [Potts and Domb 1952]. Spatial random partition models in this direction are a growing research area, including Markov random field (MRF) with the product partition model (PPM) [Pan et al. 2020], with DP [Orbanz and Buhmann 2007, Xu et al. 2016], with Pitman–Yor process (PY) [Li et al. 2020] and with mixture of finite mixtures (MFM) [Hu et al. 2020, Zhao et al. 2020]. Precisely, within the BNP framework, we focus on the class of Gibbs-type random partitions [Cerqueti 2008, Lijoi and Prünster 2010, Pitman 2006], motivated by their comprise between tractable predictive rules and richness of the predictive structure, including important cases, such as the DP [Ferguson 1973], PY [Perman et al. 1992], Pitman [1996], and MFM [Miller and Harrison 2018]. The Potts-Gibbs models induce a distribution on the partition \( \pi_p = \{C_1, \ldots, C_M\} \) of \( p \) pixels into \( M \) nonempty, mutually exclusive, and exhaustive subsets \( C_1, \ldots, C_M \) such that \( \bigcup_{C_i \in \pi_p} C = \{1, \ldots, p\} \). The model can be summarised as:

\[
\Pr(\pi_p) \propto \exp \left( \sum_{j \sim k, j < k} w_{jk} \mathbb{1}_{z_j = z_k} \right) \bigg/ \prod_{m=1}^M W_m(\phi),
\]

where \( z_j \in \{1, \ldots, M\}, j \sim k \) means that \( j \) and \( k \) are neighbors, and \( \mathbb{1}_{z_j = z_k} \) equals to 1 if \( j \) and \( k \) in the same cluster and 0 otherwise. In the following, we assume the spatial locations lie on a rectangular lattice with first-order neighbors and a common coupling parameter \( \nu \) for all neighbor pairs; a higher value of \( \nu \) encourages more spatial
We develop a Gibbs sampler to simulate from the posterior with a generalized Swendsen-Wang (GSW) algorithm to ensure mixing. Poor mixing can be seen in single-site Gibbs sampling Geman and Geman. To identify relevant regions, we use heavy tailed priors for the unique values \( \alpha \) and \( \eta \) and selection consistency Song and Liang [2017]: a 1-shrinkage prior is used, motivated by its computational efficiency and nearly optimal contraction rate. Specifically, a constant. Existing cluster and MFM models. and focus our study on three cases 1) DP with concentration parameter \( \alpha > 0 \); 2) PY with discount parameter \( \delta \in [0, 1) \) and concentration parameter \( \alpha > -\delta \); and 3) MFM with parameter \( \gamma > 0 \) (larger values encouraging more equally sized clusters) and a distribution \( P_L(\cdot|\lambda) \) with parameter \( \lambda \) related to the prior on the number of clusters. The \( \{V_p(M) : p \geq 1, 1 \leq M \leq p\} \) denotes the set of non-negative weights, which solves the backward recurrence relation \( V_p(M) = (p - \delta M)V_{p+1}(M) + V_{p+1}(M + 1) \) with \( V_1(1) = 1 \). Table 1 describes the \( V_p(M) \) and \( W_m(\phi) \) for DP, PY and MFM models.

### 2.3 Shrinkage Prior

To identify relevant regions, we use heavy tailed priors for the unique values \((\beta_1^*, \ldots, \beta_M^*)\) of \((\beta(s_1), \ldots, \beta(s_p))\). Specifically, a \( t \)-shrinkage prior is used, motivated by its computational efficiency and nearly optimal contraction rate and selection consistency Song and Liang [2017]:

\[
\sigma^2 \sim IG(a_\sigma, b_\sigma), \\
(\beta_m^*) | \sigma^2 \sim t_{s, \sigma^2}, \quad \text{for all } m = 1, \ldots, M,
\]

where \( t_{s, \sigma^2} \) denotes \( t \)-distribution with degree of freedom \( s \) and scale parameter \( \sigma^2 \). For posterior inference, the \( t \)-distribution [2] is rewritten as a hierarchical inverse-gamma scaled Gaussian mixture,

\[
\sigma^2 \sim IG(a_\sigma, b_\sigma), \\
\eta_m^* \sim IG(a_\eta, b_\eta), \\
(\beta_m^*) | \sigma^2, \eta_m^* \sim N(0, \eta_m^* \sigma^2), \quad \text{for all } m = 1, \ldots, M,
\]

where \( a_\eta \) and \( b_\eta \) are the shape and scaling parameter of the mixing distribution for each \( \eta_m^* \) respectively with \( \nu = 2a_\eta \) and \( s = \sqrt{b_\eta/a_\eta} \).

### 3 Inference

We aim to infer the posterior distribution of the parameters based on the proposed Potts-Gibbs SIR model:

\[
y_i | \mu, \beta^*, \pi_p, \sigma^2 \sim N(w_i^T \mu + x_i^T \beta^*, \sigma^2), \quad \text{for all } i = 1, \ldots, n,
\]

\[
\mu | \sigma^2 \sim N(m_\mu, \sigma^2 \Sigma_\mu),
\]

\[
\beta^* | \eta^*, \sigma^2 \sim N(0, \sigma^2 \Sigma_{\beta}),
\]

\[
\sigma^2 \sim IG(a_\sigma, b_\sigma), \\
\eta_m^* \sim IG(a_\eta, b_\eta), \quad \text{for all } m = 1, \ldots, M,
\]

\[
\pi_p \sim \text{Potts-Gibbs}(v, \phi),
\]

where \( x_{im}^* = \sum_{j=1}^p x_{ij} \mathbb{1}(j \in C_m)/\sqrt{|C_m|} \) represents the total value, e.g. volume in the \( m \)th region of the image, \( m_\mu = (m_{\mu_1}, \ldots, m_{\mu_d}), \Sigma_\mu = \text{diag}(c_{\mu_1}, \ldots, c_{\mu_d}) \), and \( \Sigma_{\beta} = \text{diag}(\eta_{\beta_1}, \ldots, \eta_{\beta_M}) \). Note that when defining \( x_{im}^* \), we rescale by the square root of cluster size, which is equivalent to rescaling the variance of \( \beta_m^* \) by the cluster size, encouraging more shrinkage for larger regions.

We develop a Gibbs sampler to simulate from the posterior with a generalized Swendsen-Wang (GSW) algorithm to draw samples from the Potts-Gibbs model. Poor mixing can be seen in single-site Gibbs sampling Geman and Geman.
We study through simulations the performance of the proposed model and compare it with Ising-DP Li et al. [2015]. We minimise the posterior expected Variation of Information (VI) Wade and Ghahramani [2018].

shown in Figures 1 - 2. For each experiment, we summarise the posterior of the clustering structure of the data sets by not considering other covariates, due to the high correlation between the pixel labels. The SW algorithm Swendsen and Wang [1987] addresses this by forming nested clusters of neighbouring pixels, then updating all of the labels within a nested cluster to the same value. The generalisation of the technique for standard Potts models to generalised Potts-partition models is called GSW Xu et al. [2016]. At each step of the algorithm, we proceed through the following steps:

1. Sample the image partition \( \pi_p \) given \( \eta^* \) and the data (with \( \beta^*, \mu, \sigma^2 \) marginalized). GSW is used to update simultaneously nested groups of pixels and hence improve the exploration of the posterior. The algorithm relies on the introduction of auxiliary binary bond variables, where \( r_{jk} = 1 \) if pixels \( j \) and \( k \) are bonded, otherwise 0. The bond variables define a partition of the pixels into nested clusters \( A_1, \ldots, A_O \), where \( O \) denotes the number of nested clusters and each \( A_m \subseteq C_m \) for some \( m = 1, \ldots, M \). For each neighbor pair \( j \sim k \) for \( 1 \leq j < k \leq p \), we sample the bond variables as follows, \( r_{jk} \sim \text{Ber}(1 - \exp(-\nu_{jk}\zeta_{jk}1_{j=Z_k})) \), where we define \( \zeta_{jk} = \kappa \exp(-\tau d(\beta_j, \beta_k)) \) with \( \beta_j \) denoting the estimated coefficient from univariate regression on the \( j \)th pixel and \( \kappa, \tau \) are the tuning parameters of the GSW sampler. Notice that the algorithm reduces to single-site Gibbs when \( \kappa = 0 \), and recovers classical SW when \( \kappa = 1 \) and \( \tau = 0 \).

As we are dealing with non-conjugate priors, we update the cluster assignment by extending Gibbs sampling with the addition of auxiliary parameters, which is widely known as Algorithm 8 Neal [2000]. We denote by \( A_o \) the current nested cluster, \( C_1^{-A_o}, \ldots, C_M^{-A_o} \) the clusters without nested cluster \( A_o \); \( M^{-A_o} \) the number of distinct clusters excluding \( A_o \), and \( h \) the number of number of auxiliary variables. For each nested cluster \( A_o \), it is assigned to an existing cluster \( m = 1, \ldots, M^{-A_o} \) or a new cluster \( m = M^{-A_o} + 1, \ldots, M^{-A_o} + h \) with probability as follows,

\[
\Pr(A_o \in C_m^{-A_o} | \cdots) \propto \frac{\Gamma(\lceil C_m^{-A_o} \rceil + |A_o| - \delta)}{\Gamma(\lceil C_m^{-A_o} \rceil - \delta)} \Pr(y | \pi_p^{A_o \rightarrow m}, \eta^*) \prod_{\{i,j\} \in A_o, k \in C_m^{-A_o}, r_{ijk} = 0} \exp\{\nu_{ijk}(1 - \zeta_{ijk})\}, \quad \text{for } C_m^{-A_o} \in \pi_p^{-A_o},
\]

where \( \Pr(y | \pi_p^{A_o \rightarrow m}, \eta^*) \) and \( \Pr(y | \pi_p^{A_o \rightarrow M + 1}, \eta^*) \) denote the marginal likelihood of data obtained by moving \( A_o \) from its current cluster to existing clusters or newly created cluster respectively. Before updating the cluster assignments, we sample the nested clusters and compute the volume of each nested cluster for all images, with computational cost \( \mathcal{O}(np) \). When updating the cluster assignments, the marginal likelihood dominates the computational cost, as it involves inversion and determinants of \( (M + q) \times (M + q) \) matrices and updating the sufficient statistics for every nested cluster and every outer cluster allocation, i.e. the cost is \( \mathcal{O}([\lceil M + q \rceil^3 + n[M + q])M) \).

2. Sample \( \beta^*, \mu, \sigma^2 \) jointly given the partition \( \pi_p, \eta^* \) and the data. Notationally, we reformulate \( \tilde{x}_i = (w_i^T, \tilde{x}_i^T)^T \) and \( \beta = (\mu^T, \beta^T)^T \). We define \( \tilde{X} \) be the matrix with rows equal to \( \tilde{x}_i^T \). The corresponding full conditional for \( \beta \) and \( \sigma^2 \) is

\[
\sigma^2 \mid \cdots \sim \text{IG}(\hat{a}_\sigma, \hat{b}_\sigma),
\]

\[
\beta \mid \sigma^2, \cdots \sim \text{N}(\hat{m}_\beta, \sigma^2 \hat{\Sigma}_\beta),
\]

where \( \hat{\Sigma}_\beta = (\Sigma_\beta^{-1} + \tilde{X}^T \tilde{X})^{-1}, \hat{m}_\beta = \hat{\Sigma}_\beta (\Sigma_\beta^{-1} m_\beta + \tilde{X}^T y), \) and \( \text{IG}(\hat{a}_\sigma, \hat{b}_\sigma) \) denotes the inverse-gamma distribution with updated shape \( \hat{a}_\sigma = a_\sigma + n/2 \) and scale \( \hat{b}_\sigma = b_\sigma + 1/2 + (\beta_m^2)/(2\sigma^2) \).  

3. Sample \( \eta^* \) given \( \beta^* \). The corresponding full conditional for each \( \eta^*_m \) is an inverse-gamma distribution with updated shape \( \hat{a}_\eta = a_\eta + 1/2 \) and scale \( \hat{b}_\eta = b_\eta + (\beta_m^2)/(2\sigma^2) \):

\[
\eta^*_m \mid \cdots \sim \text{IG}(\hat{a}_\eta, \hat{b}_\eta), \quad \text{for } m = 1, \ldots, M.
\]

4 Numerical Studies

We study through simulations the performance of the proposed model and compare it with Ising-DP Li et al. [2015]. We consider 2D images in this simulation. The \( n = 300 \) images are simulated on a two dimensional grid of size \( 10 \times 10 \), with spatial locations \( s_j = (s_{j1}, s_{j2}) \in \mathbb{R}^2 \) for \( 1 \leq s_{j1}, s_{j2} \leq 10 \). For simplicity’s sake, we include an intercept but do not consider others covariates, \( w_j \). We concentrate on the two simulation scenarios with true \( M = 2 \) and \( M = 5 \) as shown in Figures 1-2. For each experiment, we summarise the posterior of the clustering structure of the data sets by minimising the posterior expected Variation of Information (VI) Wade and Ghahramani [2018].
5 Conclusion

We have developed novel Bayesian scalar-on-image regression models to extract interpretable features from the image by clustering and leveraging the spatial coordinates of the pixels/voxels. To encourage groups representing spatially contiguous regions, we incorporate the spatial information directly in the prior for the random partition through Potts-Gibbs random partition models. We have shown the potential of Potts-Gibbs models in detecting the correct cluster structure on simulated data sets. In our experiments, the hyperparameters of the Potts-Gibbs model were determined via a simple grid search on selected combinations of hyperparameters. However, future work will consist of investigating the influence of the various parameters inherent to the model and guidelines and tools to determine hyperparameters. The model will then be applied to real images, e.g. neuroimages. Motivated by examining and identifying brain regions of interest in Alzheimer’s disease, we will use MRI images obtained from the Alzheimer’s Disease Neuroimaging Initiative (ADNI) database [www.adni-info.org]. The proposed SIR model will be extended to classification problems through the GLM framework.
Figure 2: Figures on the upper and bottom row showing the true and estimated coefficient matrix of the simulated data sets for scenario 2 under each model.

| Scenario 1 | ARI | VI | MSE       | MSPE       | M       |
|------------|-----|----|-----------|------------|---------|
| Potts-DP   | 1.0 (0.004) | 0.001 (0.010) | 1.33e-4 (5.59e-4) | 4.215 (0.057) | 2.019 (0.138) |
| Potts-PY   | 1.0 (0.004) | 0.001 (0.009) | 1.03e-4 (8.73e-5) | 4.213 (0.052) | 2.015 (0.122) |
| Potts-MFM  | 0.999 (0.007) | 0.001 (0.014) | 1.01e-4 (8.37e-5) | 4.209 (0.052) | 2.007 (0.081) |
| Ising-DP   | 0.307 (0.079) | 1.386 (0.154) | 0.807 (0.011) | 145.912 (10.051) | 4.575 (1.340) |

| Scenario 2 | ARI | VI | MSE       | MSPE       | M       |
|------------|-----|----|-----------|------------|---------|
| Potts-DP   | 0.621 (0.060) | 1.160 (0.211) | 0.246 (0.064) | 7.754 (2.653) | 6.722 (0.901) |
| Potts-PY   | 0.713 (0.050) | 1.006 (0.147) | 0.157 (0.035) | 0.868 (0.168) | 6.882 (1.090) |
| Potts-MFM  | 0.830 (0.036) | 0.599 (0.133) | 0.093 (0.014) | 0.850 (0.122) | 5.232 (0.475) |
| Ising-DP   | 0.038 (0.021) | 3.990 (0.159) | 0.980 (0.025) | 3.641 (0.526) | 15.542 (1.554) |

Table 2: Mean and standard deviation of the posterior of adjusted Rand index (ARI), variation information (VI), mean squared error (MSE), mean squared prediction error (MSPE), and number of clusters for each scenario under each model.

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