Inference tools for Markov Random Fields on lattices: The R package mrf2d

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Abstract

Markov random fields on two-dimensional lattices are behind many image analysis methodologies. mrf2d provides tools for statistical inference on a class of discrete stationary Markov random field models with pairwise interaction, which includes many of the popular models such as the Potts model and texture image models. The package introduces representations of dependence structures and parameters, visualization functions and efficient (C++ based) implementations of sampling algorithms, common estimation methods and other key features of the model, providing a useful framework to implement algorithms and working with the model in general. This paper presents a description and details of the package, as well as some reproducible examples of usage.

Keywords: Markov random fields, image analysis, R, Gibbs random fields, Potts model, texture.

1. Introduction

A Markov Random Field (MRF) is a generalization of the well-known concept of a Markov Chain where variables are indexed by vertices of a graph instead of a sequence and the notion of memory is substituted by the neighborhood (edges) of that graph. Markov Random Fields on lattices, or more generally, Gibbs distributions, have been studied in Statistical Mechanics as models for interacting particle systems. They range from the very simple Ising model (or its generalization Potts model) with pairwise nearest-neighbor interaction to models with more complex interaction types, presenting long-range and/or higher-order interaction. For an introduction to the subject we refer to Liggett (2012) and references therein.

A finite 2-dimensional lattice is a direct representation of pixel positions on a digital image. Geman and Geman (1984) make an analogy between image models and statistical mechanics systems, introducing probability-based computational methods for image restoration under a specific type of noise. Higher-order dependence structures are also described, for example, interactions with pixels more distant than nearest-neighbors. Cross and Jain (1983) use MRFs with special interaction structures to model texture images.

Many modern image analysis methodologies in statistics and machine learning are grounded on Markov Random Field theory and the local dependence characteristic of image data. Common tasks in image analysis involve image segmentation (Zhang, Brady, and Smith 2001; Kato and Pong 2006; Roche, Ribes, Bach-Cuadra, and Krüger 2011; Cao, Zhou, Xu, Meng, Xu, and Paisley 2018; Ghamisi, Maggiori, Li, Souza, Tarablaka, Moser, De Giorgi, Fang,
Chen, Chi et al. (2018), texture synthesis (Gimel’farb 1996; Freeman and Liu 2011; Verstegen, Gimel’farb, and Riddle 2016) and statistical modeling (Derin and Elliott 1987; Guillot, Rajaratnam, and Emile-Geay 2015; Freguglia, Garcia, and Bicas 2020) all of which can be achieved with the use of MRFs. Some basic references are Blake, Kohli, and Rother (2011) and Kato, Zerubia et al. (2012).

In this paper, when we refer to a MRF, we consider the particular case where variables are indexed by points of a 2-dimensional lattice, not a general graph structure. The regular grid naturally creates a spatial structure and notions of distance and direction for the variables, allowing models to be specified based on this spatial structure (see Besag 1974, for examples).

Parametric inference based on maximum likelihood for such models is difficult, even for the simple models, because of the intractable constant that appears in the likelihood. Inference for the simplest non-trivial case of the Ising model was first studied by Pickard (1987) and continues to present challenges, see for example Bhattacharya, Mukherjee et al. (2018). On the other hand, while there is a continuous development of methodologies used in MRFs in the theoretical field, implementing new algorithms is a challenge in practice, mostly due to the high-dimensionality of the problem and the complexity of the data structures required to represent the data in this type of problem. An overview of this topic, mainly from the Bayesian perspective, can be found in Winkler (2012).

Most methodologies developed are based on Monte-Carlo Markov Chain methods, thus simple tasks like evaluating pairs of pixels or sampling individual pixels need to be repeated millions or billions of times in iterative methods, depending on the image size, making an efficient implementation of such methods one of the main demands for researchers of the topic.

R (R Core Team 2020) is one of the most used programming languages among Statistics researchers, what makes the existence of good packages important for any field of Statistics. In a general context (considering the definition of MRFs with general undirected graphs), packages like graph (Gentleman, Whalen, Huber, and Falcon 2020) and network (Butts 2008) provides tools for representation and manipulation of graph structures which can be used for constructing and visualizing graph-based models. Different versions of graph-based MRFs appear in many packages. For example, the CRF package (Wu 2019) has inferential tools Markov random fields with pairwise and unary interactions and their hidden MRF version, MRFcov (Clark, Wells, and Lindberg 2018) allows inference for the interaction parameter of between nodes of a graph considering covariates and gamlss.spatial (De Bastiani, Rigby, Stasinopoulos, Cysneiros, and Uribe-Opaiz 2018) allows fitting Gaussian Markov random fields in a spatial context, similar to INLA (Rue, Martino, and Chopin 2009) and mgcv (Wood 2017).

Outside of the R ecosystem, there are powerful software in C++ used for image analysis related to Markov random fields, such as the DGM library (Kosov 2013) and densecrf (Krähenbühl and Koltun 2011), which also has a Python wrapper (Beyer 2015), and can be used for a variety of tasks and use extremely efficient computational methods.

For discrete MRFs on lattice data, closer to what is proposed in mrf2d, there are some R packages available. The potts package (Geyer and Johnson 2020), implements simulation algorithms and parameter estimation via Composite-Likelihood for a Potts model with nearest-neighbor interactions only. PottsUtils (Feng and Tierney 2018) also implements simulation and tools for computing normalization constants in one, two and three-dimensional Potts model. The package bayesImageS (Moores, Nicholls, Pettitt, Mengersen et al. 2018)
provides Bayesian image segmentation algorithms considering Gaussian mixtures driven by Hidden Potts models with slightly more complex interaction neighborhood. GiRaF (Stoehr, Pudlo, and Friel 2016) allows calculation on, and sampling from general homogeneous Potts model. The Pottslab (Storath and Weinmann 2014) package for MATLAB also provides image segmentation algorithms using the Potts model, including for multivariate-valued data.

Although the available packages for discrete-valued MRFs offer efficient implementations of their methods, they do not provide an interface that allows simple extensions to different cases, for example, different interaction types for different positions and sparse long-range interaction neighborhoods. Some of the algorithms used also rely on specific characteristics of the specific setups they consider and cannot be applied more generally.

The mrf2d package (Freguglia 2020) provides a complete framework for statistical inference on discrete-valued MRF models on 2-dimensional lattice data, where all the elements used by algorithms (such as conditional probabilities, pseudo-likelihood function, simulation, sufficient statistics and more) are available for the user, as well as many built-in model fitting functions. The package uses the model described in Freguglia et al. (2020) as a reference. Many other models, such as the Potts model and auto-models, are particular cases of our model obtained by including restrictions to the parameters or using specific interacting neighborhoods. These neighborhoods can be freely specified within the package and 5 families of parameter restrictions are available to cover the particular cases.

mrf2d is available on CRAN and as a development version in its git repository. These versions can be installed with

```
R> install.packages("mrf2d") # CRAN version
R> devtools::install_github("Freguglia/mrf2d") # Development version
R> library("mrf2d")
```

This paper is organized as follows. Section 2 describes the model considered in mrf2d, Section 3 presents the main functionalities of the package and details of the implementation, which are illustrated by examples in Section 4. We finish with a discussion in Section 5.

2. Model description

Let \( \mathcal{L} \subset \{i = (i_1, i_2) \in \mathbb{N}^2\} \) a finite set of locations in a two-dimensional lattice region and \( Z = \{Z_i\}_{i \in \mathcal{L}} \) a field of random variables indexed by those locations.

The main purpose of mrf2d is to provide a general framework for Markov random field models which satisfy the following assumptions:

(a) **Finite support** Each \( Z_i \) can take values in \( Z = \{0, \ldots, C\} \) for some finite \( C > 0 \).

(b) **Pairwise interactions** The probability of a complete configuration \( P(Z = z) \) can be decomposed into a product of functions of the pairs \( (z_i, z_j), i \neq j \in \mathcal{L} \).

(c) **Homogeneous interactions** The interaction between to pixels \( i \) and \( j \) is the same as for the pixels \( i' \) and \( j' \) if \( i - i' = j - j' \), i.e., the interactions depend on the relative position of a pair of pixel, not on their position in the lattice.
These assumptions are satisfied by most commonly used models in image processing. We use the representation in Freguglia et al. (2020) which expresses the probability distribution of the random field in the form of the exponential family and introduce additional constraints to parameter space and/or different dependence structures to include particular features of the model under study.

### 2.1. Homogeneous Markov Random Field with pairwise interactions

MRF models are characterized by their conditional independence property. Let \( \mathcal{N} \) a neighborhood system on \( \mathcal{L} \), then \( \mathbf{Z} \) is a Markov random field with respect to \( \mathcal{N} \) if \( Z_i \) given its neighbors \( Z_{\mathcal{N}_i} \) is conditionally independent from all other variables

\[
P(Z_i = z_i | Z_{-i}) = P(Z_i = z_i | Z_{\mathcal{N}_i}), \quad i \in \mathcal{L},
\]

where \( Z_{-i} \) denotes the set of variables \( \{Z_j, j \neq i\} \).

To start defining MRFs in an image processing context, a location of the lattice \( i \in \mathcal{L} \) will be referred as a pixel \( i \) and an observed value of the variable \( z_i \in \mathcal{Z} \) as pixel value or color.

We denote \( \mathcal{R} \subset \mathbb{Z}^2 \) a set of interacting relative positions such that, for no pair of elements \( r, r' \in \mathcal{R} \) we have \( r' = -r \) (no position in \( \mathcal{R} \) is a reflection of another). Based on \( \mathcal{R} \), we can construct a neighborhood system (interaction structure) \( \mathcal{N} \) in such way that the set of neighbors of site \( i \), \( \mathcal{N}_i \) can be represented by a graph with vertices \( \mathcal{L} \) where there is an edge connecting \( i \) and \( j \) if, and only if, \( j = i \pm r \). For example, a nearest-neighbor structure corresponds to \( \mathcal{R} = \{(1,0), (0,1)\} \).

Given an interaction structure \( \mathcal{R} \), for any relative position \( r \in \mathcal{R} \) the interactions associated to that relative position are characterized by a map \( \theta_r(\cdot, \cdot) \), \( \theta_r : \mathbb{Z}^2 \to \mathbb{R} \). For \( a, b \in \mathcal{Z} \), the value \( \theta_r(a,b) \) is called a potential.

The model in mrf2d considers a neighborhood system \( \mathcal{N} \) that connects pairs of pixel positions \( i, j \) such that \( i - j \in \mathcal{R} \). Under assumptions (a), (b) and (c), the Hammersley-Clifford theorem (Hammersley and Clifford 1971) implies that the probability function for \( \mathbf{Z} \) belongs to the exponential family and can be described by a set of natural parameters \( \theta = \{\theta_r(a,b), r \in \mathcal{R}, a, b \in \mathcal{Z}\} \),

\[
P(\mathbf{Z} = \mathbf{z}) = \frac{1}{\zeta_{\theta}} e^{H(\mathbf{z}, \theta)},
\]

where

\[
H(\mathbf{z}, \theta) = \sum_{r \in \mathcal{R}} \sum_{i,j \in \mathcal{L}} \theta_r(z_i, z_j) 1_{(j = i + r)} \text{ and } \zeta_{\theta} = \sum_{\mathbf{z}'} e^{H(\mathbf{z}', \theta)}.
\]

Figure 1 illustrates how the function \( H(\mathbf{z}, \theta) \) is computed for an example interaction structure \( \mathcal{R} \) and a field \( \mathbf{z} \).

Note that adding a constant a constant \( c_r \) to the potentials associated with a relative position \( r \in \mathcal{R} \) results in the same probability because the constant cancels when dividing by \( \zeta_{\theta} \). Thus, constraints for the potentials \( \theta_r(a,b) \) are necessary to obtain identifiability in the model. We consider \( \theta_r(0,0) = 0 \) for all relative positions \( r \), which ensures identifiability and also gives an interpretation for interactions in terms of the pair \((0,0)\): \( \theta_r(a,b) < 0 \) (resp. \( > 0 \)) means that the pair \((a,b)\) is less (resp. more) likely to appear in a pair with relative position \( r \) than \((0,0)\).
Interaction Structure

\[ \mathcal{R} = \{(1,0), (0,1), (2,2)\} \]

Data

\[ z = \begin{pmatrix} 0 & 0 & 2 \\ 1 & 2 & 1 \\ 0 & 2 & 0 \end{pmatrix} \]

Pairwise contributions to \( H(z, \theta) \)

\[
\begin{array}{c|c|c}
(0,2) & \theta_{(0,2)}(0,0) + \theta_{(0,1)}(0,0) + \theta_{(2,2)}(0,2) & \\
1 & 2 & 1 \\
0 & 2 & 0 \\
\end{array}
\]

\[
\begin{array}{c|c|c}
(0,2) & \theta_{(0,2)}(1,0) + \theta_{(0,1)}(1,0) & \\
1 & 2 & 1 \\
0 & 2 & 0 \\
\end{array}
\]

\[
\begin{array}{c|c|c}
(0,2) & \theta_{(0,2)}(2,0) + \theta_{(0,1)}(2,0) & \\
1 & 2 & 1 \\
0 & 2 & 0 \\
\end{array}
\]

\[
\begin{array}{c|c|c}
(0,2) & \theta_{(0,2)}(0,0) + \theta_{(0,1)}(2,0) & \\
1 & 2 & 1 \\
0 & 2 & 0 \\
\end{array}
\]

\[
\begin{array}{c|c|c}
(0,2) & \theta_{(0,2)}(1,0) + \theta_{(0,1)}(2,1) & \\
1 & 2 & 1 \\
0 & 2 & 0 \\
\end{array}
\]

Figure 1: Example of interaction structure with three relative positions and example field on a 3 by 3 lattice (left) and contributions of each interacting pair to \( H(z, \theta) \) (right).

**Potts Model as a particular case** The Potts model (Potts 1952) is one of the most important MRF model used in image segmentation because it can assign higher probability for equal-valued pairs of nearest-neighbors, creating large regions of pixels with the same values. The model has a single parameter \( \phi \) that is interpreted as the inverse temperature in a mechanical statistics context.

A standard Potts Model can be expressed as (2) with the function \( H(z, \theta) \) taking the form

\[
\phi \sum_{(i,j) : ||i-j||=1} I_{(z_i \neq z_j)}. \tag{4}
\]

Assumptions (a), (b) and (c) are satisfied, thus, we can rewrite (4) in terms of an interaction structure \( \mathcal{R} \) and potentials \( \theta \) by noticing

- The set \( i,j : ||i-j|| = 1 \) are vertical and horizontal pairs of neighbors, therefore, the interaction structure \( \mathcal{R} \) is the set \{ \( (1,0), (0,1) \) \}.

- The potential \( \theta_r(a,b) \) is equal to \( \phi \) if \( a \neq b \) and 0 otherwise, regardless of \( r \). The constraint \( \theta_r(0,0) = 0 \) is satisfied in this definition. Therefore, we have the parameter restriction

\[
\theta_r(a,b) = \phi I_{(a \neq b)}
\]

for all \( r \in \mathcal{R} \).
This parameter restriction corresponds to the "onepar" family described in Section 3.2.

2.2. Important elements of the model

The main inference challenge for MRFs lies in the normalizing constant $\zeta_{\theta}$ appearing in (2). It cannot be evaluated in practice as it requires summing over $|\mathcal{L}|$ possible field configurations and there is no analytical expression for it, except for trivial cases, leading to an intractable likelihood.

Being unable to evaluate the likelihood function hinders the use of most statistical methods. Inference under intractable likelihoods have been developed over the years. The main studies involve using conditional probability-based functions, like pseudo-likelihood (Jensen and Künsch 1994, for example) and Monte-Carlo methods (Geyer and Thompson 1992; Møller, Pettitt, Reeves, and Berthelsen 2006, for example).

Although there is a wide variety of inferential methods available, most of them are built using the same pieces of the model. Thus, having access to each of these pieces is necessary to implement algorithms. We highlight important characteristics of the model available in mrf2d that are used by inference methods.

Conditional Probabilities  A consequence of the Markov property (conditional independence) is a simple expression for conditional probabilities. $H(z, \theta)$ is a sum of terms that only depends on pairs of pixel values, which implies that all terms not involving position $i$ cancel out when evaluating $P(Z_i | Z_{\neq i})$. Define the part of the sum that involves the pixel in position $i$ as

$$h_i(k | z) = \sum_{r \in \mathcal{R}} \theta_r(k, z_{i+r}) + \sum_{r \in \mathcal{R}} \theta_r(z_{i-r}, k).$$

The conditional probability of $Z_i = k$ given all other locations, $P(Z_i = k | Z_{\neq i})$, is then given by the standard softmax of $h_i(k | z)$,

$$P(Z_i = k | Z_{\neq i} = z_{\neq i}) = \frac{e^{h_i(k | z)}}{\sum_{k'} e^{h_i(k' | z)}}. \tag{6}$$

Pseudo-likelihood function  The pseudo-likelihood function (Besag 1974, 1975) is defined as the product of conditional probabilities of each variable given all other variables of a random field,

$$PL(\theta; z) = \prod_{i \in \mathcal{L}} P(Z_i = z_i | Z_{\neq i} = z_{\neq i}) = \prod_{i \in \mathcal{L}} \frac{e^{h_i(z_i | z)}}{\sum_{k'} e^{h_i(k' | z)}}. \tag{7}$$

In the special case of an independent field, it is equivalent to the likelihood function. Notice that the pseudo-likelihood function does not depend on the intractable normalizing constant and (7) is numerically equivalent to a logistic regression problem where each pixel values corresponds to independent observations and the interacting pixel values are covariates with coefficients corresponding to the associated potentials.
Generating MRFs via Gibbs Sampler  While exact sampling from dependent and high-dimensional processes is a challenging task overall, the conditional independence of MRFs simplifies the implementation of the Gibbs Sampler algorithm (Geman and Geman 1984). In the Gibbs Sampler algorithm, each pixel value is updated conditionally to the current state of its neighbors and a Gibbs Sampler cycle consists of updating each pixel exactly one time.

To avoid introducing any kind of bias due to updates order, a random permutation of $\mathcal{L}$ is drawn to define the order in which pixels are updated at each cycle. After running a suitable number of cycles in Algorithm 1, the distribution of the resulting field sampled in the process is approximately the joint distribution of the MRF.

Algorithm 1: Approximate Sampling algorithm for MRFs using $T$ steps of Gibbs Sampler.

| Initialize $z$ with a starting configuration $z = z^{(0)}$; |
| Initialize the iteration counter $t = 0$; while $t \leq T$ do |
| Sample $\{i^{(1)}, i^{(2)}, \ldots, i^{(|\mathcal{L}|)}\}$ a random permutation of the pixel positions $\mathcal{L}$; |
| for $j$ in $1, \ldots, |\mathcal{L}|$ do |
| Update $z_{i(j)}$ conditional to the rest of the field $z_{-i(j)}$ with probabilities from |
| Equation (6); |
| end |
| $t = t + 1$; |
| Result: output the final configuration $z$. |

Sampling a field conditional to a subset of pixel values can be achieved with the same algorithm by skipping the updates for those pixels which are being conditioned on.

There exists faster mixing algorithms for particular cases such as Swendsen-Wang algorithm (Wang and Swendsen 1990), but they require specific conditions from the model and/or particular implementations to be efficient. Therefore, we keep the Gibbs Sampler as the method of choice in this work due to its generalization ability as it only requires computing conditional distributions, despite its slower mixing times in some scenarios.

Sufficient statistics  An important computational consequence of the model assumptions is the fact that, in order to evaluate the probability (or likelihood) function for a particular observed field $z$, it is not necessary to determine the values of each pixel individually, but only the co-occurrence counts each relative position $r \in \mathcal{R}$. $H(z, \theta)$ can be rewritten as

$$H(z, \theta) = \sum_{r \in \mathcal{R}} \sum_{a=0}^{C-1} \sum_{b=0}^{C-1} \theta_r(a, b) n_{a,b,r}(z),$$

where $n_{a,b,r}(z) = \sum_{i \in \mathcal{L}} \mathbbm{1}_{(z_{i+1} = a, z_i = b)}$ is the count of occurrences of the pair $(a, b) \in \mathcal{Z}^2$ in pairs of pixels with relative position $r$. Therefore,

$$S_{\mathcal{R}}(z) = \{n_{a,b,r}(z), a, b \in \mathcal{Z}, r \in \mathcal{R}\}$$

is a vector of sufficient statistics, where each component $n_{a,b,r}(z)$ is associated with a corresponding potential $\theta_r(a, b)$. Gimel’farb (1996) calls this sufficient statistic the co-occurrence histogram.
Parameter constraints reduce the dimension of the sufficient statistic. Our identifiability constraint $\theta_r(0,0) = 0$ implies that all $n_{0,0,r}(z)$ are excluded from $S_R(z)$ and equality constraints require aggregating (sum) co-occurrence counts to match the parameter dimension. We shall keep the same notation for the constrained version of the sufficient statistics $S_N(z)$ and potentials $\theta$.

The main advantages of the representation with sufficient statistics are the reduced memory usage in Monte-Carlo methods and a convenient representation of $H(z, \theta)$ with an inner product that simplifies dealing with likelihood ratios as in Geyer and Thompson (1992),

$$H(z, \theta) = \langle S_N(z), \theta \rangle. \quad (9)$$

### 2.3. Gaussian mixtures driven by Hidden MRFs

Another class of models present in the image processing field are Hidden Markov Random Field models (HMRFs). The hidden version considers a latent (unobserved) process, denoted $Z$ and an observed field, denoted $Y$, where $Z$ is distributed as a MRF and the distribution of $Y|Z$ is reasonably simple.

In this type of modeling, $Z$ is often considered the “true” image and $Y$ is a noisy image. Therefore, the goal of the analysis in this context is usually to recover the underlying field. Note that for models like the one in this work, where $Z$ has finite support, the hidden field defines a segmentation of the image, making it a suitable approach for image segmentation.

In mrf2d, we provide built-in tools for the case where $Y|Z$ is a finite Gaussian mixture where mixture components are driven by the hidden field. Additional covariates can also be included as fixed effects for the mean,

$$Y_i|Z_i = a \sim N(\mu_a + \mathbf{x}_i \top \beta, \sigma_a^2), \quad a = 0, 1, \ldots, C. \quad (10)$$

Observed values $Y$ are also considered independent given the latent field, leading to the conditional density

$$f(y|Z = z) = \prod_{i \in L} \frac{1}{\sqrt{2\pi \sigma_{z_i}^2}} \exp \left( \frac{(y_i - \mu_{z_i} - \mathbf{x}_i \top \beta)^2}{2\sigma_{z_i}^2} \right) \quad (11)$$

and the complete likelihood function

$$L_\theta(\beta, \mu_a, \sigma_a, a = 0, \ldots, C; y, z) = \frac{1}{\xi_\theta^{(H(z, \theta))}} \prod_{i \in L} \frac{1}{\sqrt{2\pi \sigma_{z_i}^2}} \exp \left( \frac{(y_i - \mu_{z_i} - \mathbf{x}_i \top \beta)^2}{2\sigma_{z_i}^2} \right) \quad (12)$$

Inference for this models involves estimating the parameters $(\mu_k, \sigma_k)_{k=0,1,\ldots,C}$ and $\beta$ associated with the Gaussian Mixture and predicting the labels of the latent field $z$ simultaneously. Bayesian methods and the EM algorithm are the most common approaches. The parameters of the latent field distribution $\theta$ are fixed a priori and considered tuning hyper-parameters of
3. Using the Package

3.1. Model representation

The model described in Section 2 can be completely characterized by three components: the random field \( z \), the interaction structure \( R \) and the potentials \( \theta \). Additionally, \( y \) and the mixture parameters \((\mu_k, \sigma_k^2)_{k=0,...,C}\) are included in Hidden MRFs.

A consistent representation of each component is provided in the package so that inputs and outputs of built-in functions, as well as methods the user may implement, are compatible and usable in the analysis pipeline. Representations are described in Table 1.

| Model Component | Function | Representation in mrf2d |
|-----------------|----------|------------------------|
| \( z \): Discrete-valued field | \( Z \) | A matrix object with values in \( \{0, \ldots, C\} \), where \( Z[w,q] \) represents the pixel value in position \( (w,q) \) of the lattice. NA values are used for positions that do not belong to \( \mathcal{L} \) when it is not a rectangular region. |
| \( y \): Countinuous-valued field | \( Y \) | A matrix object with real values, where \( Y[u,v] \) represents the pixel value in position \( (u,v) \) of the lattice. NA values are used for positions that do not belong to \( \mathcal{L} \) when it is not a rectangular region. |
| \( R \): Interaction structure | \( \text{mrfi} \) | An object of the S4 class \text{mrfi}. It can be created with the \text{mrfi}() function. |
| \( \theta_r(a,b) \): Array of potentials | \( \text{theta} \) | A three-dimensional array object with dimensions \((C+1) \times (C+1) \times |\mathcal{R}| \). For a pair of values \((a,b)\) and the \( s \)-th interacting position \( r_s \) of \( \mathcal{R} \), the corresponding potential is mapped at \( \text{theta}[a+1, b+1, s] \). |

**Random fields \( z \) and \( y \).** Realizations of a random fields \( z \) and \( y \) are represented by simple matrix objects with dimension \( N \times M \), where \( N \geq \max_{i_1} (i_1, i_2) \in \mathcal{L} \) and \( M \geq \max_{i_2} (i_1, i_2) \in \mathcal{L} \), i.e., the maximal coordinates. This matrix represents a rectangular set of pixels that contains \( \mathcal{L} \). The value in row \( i_1 \) and column \( i_2 \) represents the observed value of the random field in position \((i_1, i_2)\): an integer in \( \{0, 1, \ldots, C\} \) for \( z \) or a real number for \( y \).

We do not require \( \mathcal{L} \) to be a complete rectangular region. Pixels which position does not belong to \( \mathcal{L} \) are be assigned the NA value.

Two functions are available for visualizing random fields: \text{dplot}() and \text{cplot}(). \text{dplot}() should be used for discrete-valued fields \( z \) while \text{cplot}() is used for continuous-valued matrices \( y \). These functions provide an alternative to base R \text{image}() function, producing elegant images in the form of ggplot objects. The main advantage is that they allow the use of the ggplot2 package (Wickham 2016) to customize the image using the grammar of graphics.
Details and examples of customization of the images produced using `ggplot2` can be found in Appendix A.

**Interaction Structures** \(\mathcal{R}\) Interaction structures are represented by objects of the S4 class `mrfi` implemented in `mrf2d`. These objects can be created with the `mrfi()` function, which has arguments `max_norm`, `norm_type` and `positions`. The interaction structure created will include all relative positions which satisfy \(||(i_1,i_2)|| \leq \text{max norm}\) for the specified norm type. `positions` can be passed as a list containing length 2 integer vectors with relative positions to include. The function automatically checks for repeated and opposite relative positions to ensure the structure is valid.

`norm_type` options are the same as R built-in `norm()` function, mainly, "1", "2" and "m" are used for \(\ell_1\), \(\ell_2\) and the maximum norm, respectively. The default is \(\ell_1\) norm.

Some examples for creating different `R` are detailed below.

- `mrfi(max_norm = 1)` creates an interaction structure with all positions with \(||(i_1,i_2)|| \leq 1\), which corresponds to a nearest-neighbor structure \(\mathcal{R} = \{(1,0),(0,1)\}\).
- `mrfi(max_norm = 0, positions = list(c(1,0), c(0,1)))` is an alternative way of specifying the same structure of the previous example.
- `mrfi(max_norm = 1, positions = list(c(2,0)))` results in the interaction structure \(\mathcal{R} = \{(1,0),(0,1),(2,0)\}\).
- `mrfi(max_norm = 1, positions = list(c(-1,0)))` results in \(\mathcal{R} = \{(0,1),(-1,0)\}\). The norm-based and position-based positions had an intersection, so the redundant position \((1,0)\) was removed. In case of opposite directions, the `positions` argument is prioritized as it was explicitly defined by the user.

An algebra of `mrfi` objects is implemented for manipulating these objects. `+` is used to perform union of two `mrfi` objects or a `mrfi` object and a numeric vector with 2 integers can be used to add a single interacting position to an existing `mrfi` object. Similarly, the `−` operator can be used to perform set difference between two `mrfi` objects or to remove a single position if a vector with 2 integers is used in the right-hand-side.

Additionally, conversion of `mrfi` objects to `list` is implemented in the `as.list()` method. Subsetting methods are also available with the "[]" and "[[ ]]" operators. These methods are particularly important for model selection algorithms, as many distinct sparse interaction structures can be obtained by using different subsets of a large reference base structure.

A `plot` method is available for `mrfi` objects. The code chunk below exemplifies the usage of plotting functions and manipulation of `mrfi` objects. The resulting plots are presented in Figure 2. The black square represents the origin position \((0,0)\), positions included in the interaction structure \(\mathcal{R}\) are represented by the dark-gray squares with black borders, while their opposite directions are the light-gray squares.

```r
R> plot(mrfi(max_norm = 1))
R> plot(mrfi(max_norm = 2, norm_type = "m") + c(4,0))
R> plot(mrfi(4) - mrfi(2))
R> plot(mrfi(6, norm_type = "m")[c(1,2,6,9,19,41)])
```
Potentials array $\theta$ The collection of potentials, $\theta_r(a, b)$, is represented by an array object with dimensions $(C + 1) \times (C + 1) \times |R|$. Rows and columns are used to map $a$ and $b$, respectively, while slices are used to map relative positions $r$. A set of potentials $\{\theta_r(a, b), a, b \in \mathbb{Z}, r \in R\}$ is always related to an interaction structure $R = \{r_1, r_2, \ldots, r_{|R|}\}$. The $i$-th slice maps the $i$-th relative position of $R$, $r_i$.

An important detail is that array indices in $R$ start at 1, while we consider our set of possible values $\mathbb{Z} = \{0, 1, \ldots, C\}$, therefore we need to shift $a$ and $b$ one position when accessing their value in the $R$ array. Figure 3 illustrates how potentials can be represented as an array in $R$ in the $C = 2$ case. Two elements are highlighted and the associated indices used to access them are shown as examples.

![Figure 3: Example of array representation of potentials with $C = 2$.](image)

3.2. Parameter restriction families

Parameter restrictions play an important role in the inference process of our Markov Random Field models. mrf2d functions support 5 families of parameter restrictions for the array of potentials to be considered in inference algorithms. They are specified by the family argument of functions to ensure the resulting output array (theta) respects those constraints. A brief description of each interaction structure is given next. Table 2 presents the mathematical
definitions, number of free parameters and an example of a slice of the array of potentials for the case with $C = 2$ in each family.

Table 2: Description of parameter restriction families.

| Family | Restriction | Free parameters | Example slice |
|--------|-------------|----------------|---------------|
| "onepar" | $\theta_r(a,b) = \phi \mathbf{1}_{a \neq b}$ | 1 | $\begin{bmatrix} 0 & \phi & \phi \\ \phi & 0 & \phi \\ \phi & \phi & 0 \end{bmatrix}$ |
| "oneeach" | $\theta_r(a,b) = \phi_r \mathbf{1}_{a \neq b}$ | $|\mathcal{R}|$ | $\begin{bmatrix} 0 & \phi_r & \phi_r \\ \phi_r & 0 & \phi_r \\ \phi_r & \phi_r & 0 \end{bmatrix}$ |
| "absdif" | $\theta_r(a,b) = \sum_{d=1}^{C} \phi_{r,d} \mathbf{1}_{|b-a| = d}$ | $|\mathcal{R}|C$ | $\begin{bmatrix} 0 & \phi_{r,1} & \phi_{r,2} \\ \phi_{r,1} & 0 & \phi_{r,1} \\ \phi_{r,2} & \phi_{r,1} & 0 \end{bmatrix}$ |
| "dif" | $\theta_r(a,b) = \sum_{d=-C,d\neq 0}^{C} \phi_{r,d} \mathbf{1}_{(b-a) = d}$ | $|\mathcal{R}|2C$ | $\begin{bmatrix} 0 & \phi_{r,1} & \phi_{r,2} \\ \phi_{r,-1} & 0 & \phi_{r,1} \\ \phi_{r,-2} & \phi_{r,-1} & 0 \end{bmatrix}$ |
| "free" | $\theta_r(0,0) = 0$ | $|\mathcal{R}|(C^2 - 1)$ | $\begin{bmatrix} 0 & \phi_{r,0,1} & \phi_{r,0,2} \\ \phi_{r,1,0} & \phi_{r,1,1} & \phi_{r,1,2} \\ \phi_{r,2,0} & \phi_{r,2,1} & \phi_{r,2,2} \end{bmatrix}$ |

"onepar" A single-parameter ($\phi$) model, where interactions depend only on the fact that values are equal or different, regardless of their relative position. This restriction corresponds to the classical Ising and Potts model.

"oneeach" The same interaction type as "onepar", but allowing different values $\phi_r$ for different interacting positions $r \in \mathcal{R}$.

"absdif" For each $r \in \mathcal{R}$, the potentials $\theta_r(a,b)$ are equal when the absolute differences of their pixel values $d = |b-a|$ are the same. Note that "absdif" is equivalent to "oneeach" when $C = 1$.

"dif" Generalizes the "absdif" family allowing opposite signal differences to have different interactions.

"free" No restrictions, except for the identifiability constraint $\theta_r(0,0) = 0$.

Families "dif" and "absdif" should only be used when pixel values are actually quantities and differences are well-defined, for example, in grayscale images with few levels, for example in Gimel'farb (1996). If relabeling the values does not change the interpretation of the problem, then these restrictions are probably not suitable.

The function \texttt{smr_array(theta, family)} can be used to transform a parameter array into a vector of appropriate length containing only the free parameters corresponding to the provided array ($\texttt{theta}$) and the restriction \texttt{family}. The opposite operation is also available as the \texttt{expand_array(theta_vec, family, mrfi, C)} function. This transformations are particularly useful for optimization problems as most functions, for example, R built-in \texttt{optim}
function requires a vector of parameters and for storing multiple vectors, for example in Monte-Carlo methods, using a simpler and less memory consuming structure.

### 3.3. Random field sampler

Being able to sample observations of Markov random fields is a key component of many inference methods that aim to avoid the intractable normalizing. In mrf2d, a complete and efficient routine to sample fields using the Gibbs Sampler algorithm described in Algorithm 1 is provided by the rmrf2d() function. Its arguments are:

- **init.Z**: The initial field configuration, or a length-2 vector with the dimensions of the field to be sampled. If the dimensions are provided, the initial configuration is randomly sampled from independent discrete uniform distributions.
- **mrfi**: A mrfi object representing the interaction structure $R$.
- **theta**: An array of potentials.
- **cycles**: The number of Gibbs Sampler cycles.
- **sub_region**: Optional argument used for non-rectangular images when init.Z is a vector with the dimensions. A logical matrix with the same dimensions as specified in init.Z. Pixels with FALSE value are not included in the image.
- **fixed_region**: Optional. A matrix with logical values. Pixel positions with TRUE value are conditioned on their initial configuration (init.Z) value and are not updated.

We illustrate the use of the sampling function below on two $200 \times 200$ fields: one without conditioning on any pixel (nothing specified in fixed_region) and one conditioned on the border values set as 0. The resulting images are presented in Figure 4.

```r
R> th <- expand_array(-1, family = "onepar", mrfi(1), C = 1)
R>
R> # Sample a field
R> z_sample <- rmrf2d(init.Z = c(200,200), mrfi = mrfi(1), theta = th)
R>
R> # Sample a field conditional to the border values being 0
R> ## Define the logical matrix for the fixed region.
R> border <- matrix(FALSE, nrow = 100, ncol = 100)
R> border[1,] <- border[100,] <- border[,1] <- border[,100] <- TRUE
R> ## Define the initial field
R> initial <- matrix(sample(0:1, 100*100, replace = TRUE),
+   nrow = 100, ncol = 100)
R> initial[border] <- 0
R> z_border <- rmrf2d(initial, mrfi = mrfi(1), theta = th,
+   fixed_region = border)
```

Fields with non-rectangular can be sampled either by passing a non-rectangular field as the init.Z argument or by using the sub_region argument and specifying the dimensions of the sampled field.
Another important feature is conditioning on a subset of pixel values. There are many situations where keeping a subset of pixels fixed during the sampling process can be useful, for example, filling a region of missing pixel values via simulation, defining boundary conditions (our model corresponds to a free boundary condition, but other types such as fixed or periodic boundary can be sampled with proper manipulation of the initial configuration and conditioning region) or performing block-wise updates of the data using conditionally independent blocks (for parallelization of algorithms).

Since the Gibbs Sampler algorithm updates each pixel value multiple times, performance is one of our main implementation concerns. To improve the performance and speed up computations considerably, the internals of the sampling function, as well as most other computationally intensive functions are written in C++ with the use of Rcpp (Eddelbuettel, François, Allaire, Ushey, Kou, Russel, Chambers, and Bates 2011) and RcppArmadillo (Eddelbuettel and Sanderson 2014) packages.

3.4. Statistical Inference in mrf2d

Inference methods for MRF models are diverse and their suitability highly depend on the type of data being analyzed. The framework provided by mrf2d can be used to implement all sorts of algorithms that are built from a common stack of components: simulation, conditional probabilities and sufficient statistics. It also provides complete built-in routines for some estimation algorithms.

Table 3 presents a list of functions available in the package that can be used to construct inference algorithms, as well as built-in functions for parameter estimation for MRF and for the Hidden MRF models defined in Section 2.3 that we describe next. The built-in inference functions return objects of class mrfout (MRF data) or hmrfout (Hidden MRF models), which contains the information about the fitted model, as well as summary and plot methods associated for interpretation of the results.

Maximum pseudo-likelihood estimation The pseudo-likelihood function in (7) can be evaluated efficiently because it does not depend on the intractable normalizing constant. A
Table 3: List of available functions used for inference in mrfd with a brief description of each one.

| Function     | Use                                                                 |
|--------------|----------------------------------------------------------------------|
| rmrf2d       | Generates samples of a MRF via Gibbs Sampler. Used for Monte-Carlo based methods. |
| cp_mrf2d     | Computes the conditional probabilities for a pixel position given its neighbors. |
| pl_mrf2d     | Computes pseudo-likelihood value for an observed field considering interaction structure mrfi and array of potentials theta. |
| cohist       | Creates the co-occurrence histogram of an observed given an interaction structure. Can be converted to a vector of sufficient statistics given a restriction family with the smr_stat function. |
| smr_array    | Conversions between array and vector representation of potentials given a parameter restriction family. |
| expand_array | Conversions between array and vector representation of potentials given a parameter restriction family. |

**Built-in inference algorithms**

| Function     | Use                                                                 |
|--------------|----------------------------------------------------------------------|
| fit_pl       | Estimates the parameter array given an observed field via pseudo-likelihood optimization. Returns a mrfout object. |
| fit_sa       | Estimates the parameter array given an observed field via Stochastic Approximation algorithm. Returns a mrfout object. |
| fit_ghm      | Fits a Gaussian Mixture driven by a given Hidden MRF model using the EM algorithm from Zhang et al. (2001). polynomial_2d and fourier_2d can be used to create polynomial and 2-dimensional Fourier basis functions, respectively, to be used as a fixed effect. Returns a hmrfout object. |

A common estimation procedure for intractable likelihood problems is optimizing the pseudo-likelihood with respect to the parameters.

$$\hat{\theta}_{PL} = \arg \max_{\theta} PL(\theta; z).$$

The function `fit_pl` from mrfd implements an optimization of the pseudo-likelihood function using R built-in `optim()` function. It handles the conversions between array and vector representation of potentials automatically, respecting the restriction family selected and returns the estimated array of potentials and maximum value of the pseudo-likelihood in logarithmic scale. The arguments of `fit_pl` are:

- `Z`: The observed random field z.
- `mrfi`: A mrfi representing an interaction structure $\mathcal{R}$.
- `family`: A parameter restriction family.
- `init`: An array with the initial configuration used in the optimization. 0 can be used to start from the independent model.
**Stochastic Approximation algorithm**  Given an observed field $z^{(0)}$, the Stochastic Approximation algorithm (Robbins and Monro 1951) seeks to create a Markov Chain of parameter vectors $\{\theta^{(t)}\}_{t \geq 1}$ that converges to the maximum likelihood estimate of $\theta$, which is the solution of the zero gradient condition $E_{\theta}(S_{R}(Z)) = S_{R}(z^{(0)})$, derived from (9).

The algorithm is defined by the recurrence

$$\theta^{(t+1)} = \theta^{(t)} + \gamma^{(t)}(S_{R}(z^{(0)}) - S_{R}(z^{(t)})),$$

(14)

where $z^{(t)}$ is a field sampled using $\theta^{(t)}$ and $\gamma^{(t)}$ is a sequence of positive constants that satisfies $\sum_{t=1}^{\infty} \gamma^{(t)} = \infty$ and $\sum_{t=1}^{\infty} (\gamma^{(t)})^2 < \infty$.

Stochastic Approximation is implemented in `mrf2d` as the `fit_sa()` function. It samples $z^{(t)}$ via Gibbs Sampler considering the previous field $z^{(t-1)}$ as the initial configuration. Periodically, the field samples are refreshed, starting from an independent discrete uniform distribution and running a greater number of Gibbs Sampler cycles, what prevents the algorithms from getting stuck in problematic field samples. Its arguments are:

- **Z** The observed field $z^{(0)}$.
- **mrfi** The interaction structure $R$.
- **family** The family of parameter restrictions considered when converting the potentials array to a vector.
- **gamma_seq** A sequence of step size values to be used as $\gamma^{(t)}$. These values are divided by the number of pixels $|L|$ internally to be invariant with respect to the image size. The typical sequence recommended is `seq(from = M, to = 0, length.out = B)`, with $M$ ranging from 0.5 to 2 and large number of iterations ($B$).
- **init** The initial array of parameters or the value 0 to start from the independent model.
- **cycles** Number of Gibbs Sampler ran between iterations.
- **refresh_each** Restarts the sample $z^{(t)}$ from a random configuration each `refresh_each` iterations.
- **refresh_cycles** When a refresh happens, how many Gibbs Sampler cycles are ran in the current parameter configuration.

Among the elements of the returned `mrfout` object, `theta` contains the estimated potential array and `metrics` a data frame with the Euclidean distances between $S_{R}(z^{(0)})$ and $S_{R}(z^{(t)})$ for each iteration. This sequence of distances is used to monitor the convergence of the algorithm as a form of diagnostics analysis.
**EM algorithm for HMRF models**  Gaussian Mixtures driven by Hidden MRFs can be fitted in mrf2d with an extension of the EM algorithm from Zhang et al. (2001) to include a fixed effect (see Freguglia et al. 2020, for details). The probabilities computed for the latent label of each pixel in the E-step are conditioned on the global maximum probability configuration of its neighbors, obtained via Iterated Conditional Modes (ICM) algorithm at each iteration (Besag 1986).

The complete algorithm is available in the fit_ghm function. Its main arguments are

- **Y**: The observed continuous-valued field y.
- **mrfi**: Interaction structure of the latent field \( \mathcal{R} \).
- **theta**: The array of potentials that defines the latent field distribution.
- **fixed_fn**: A list of functions of pixel positions \( f(i_1, i_2) \) to be used as fixed effect. Constructors for 2-dimensional polynomials and Fourier basis are available in the functions polynomial_2d and fourier_2d, respectively.
- **equal_vars**: A logical value indicating if mixture components are forced to have equal variances.
- **init_mus** and **init_sigmas**: Optional initial values of \( (\mu_a, \sigma_a)_{a=0,\ldots,C} \). If none is passed, an independent Gaussian mixture is fitted with initial values based on quantiles and the estimates of this fitted model are used as (often good) starting values in the main procedure.
- **maxiter**: Maximum number of iterations before stopping.
- **max_dist**: Defines a stopping condition for the EM algorithm. For consecutive iterations \( t \) and \( t+1 \), the absolute difference in each parameter, \( |\mu_k^{(t)} - \mu_k^{(t+1)}| \) and \( |\sigma_k^{(t)} - \sigma_k^{(t+1)}| \) are computed for \( k = 0, 1, \ldots, C \). The algorithms stops if all differences are less than max_dist.
- **icm_cycles**: Number of cycles of Iterated Conditional Modes algorithm executed in each iteration.

fit_ghm() returns a `hmrfout` object containing a `data.frame` with estimates of the mixture parameters \{\((\hat{\mu}_a, \hat{\sigma}_a), a = 0, 1, \ldots, C\)\} named `par`, the highest probability configuration of the latent field computed via ICM algorithm \( \hat{z} \) in `Z_pred`, a matrix with the estimated fixed effects \( (x_i^T \hat{\beta}) \) for each pixel in `fixed` and a matrix with the predicted mean for each pixel \( (x_i^T \hat{\beta} + \hat{\mu}_{z_i}) \) in `predicted`.

### 4. Data analysis using mrf2d

#### 4.1. Example 1: A binary image with texture-like pattern
**Description**  To illustrate the usage of mrf2d for finite-valued images, we use the object field1 available in the package, which contains a binary field with anisotropic pattern as seen in Figure 5. It is a synthetic texture image of the same type as the binary texture data presented in Cross and Jain (1983). The data can be loaded and viewed using the code chunk below.

```r
R> data("field1", package = "mrf2d")
R> dplot(field1, legend = TRUE)
```

![Figure 5: Visualization of field1.](image)

Our goal is to fit a MRF model to this data and sample images from the fitted model to evaluate if the patterns achieved in the generated data are similar to the original data. This is the typical setup of a texture synthesis problem with finite-valued images. This analysis involves three main stages: Specifying the model (interaction structure and parameter restrictions), estimating the parameters and evaluating the fitted model.

**Specifying R and parameter family** Model selection under intractability is a challenging problem because most algorithms require comparing (maximum) likelihood functions for different models, what cannot be done exactly and/or have a high computational cost for MRF models.

The main routes in the model specification stage are: using prior information of the data or problem to select what type of restrictions and interaction structure are best suited, using the most general model (e.g., no restrictions and a complex interaction structure) as in Freguglia *et al.* (2020) or using some estimation technique.

This image presents a diagonal pattern what indicates a nearest-neighbor interaction structure may not be appropriate to capture all the dependence present in the field. We first choose what kind of parameter restriction family will be considered by checking that relabeling the values $Z$ does not change the patterns in the image indicating symmetric potentials should be suited for this image, and there is a clear difference in the interactions when considering pixels in different directions, what indicates we need different types of interaction for different relative positions. These characteristics match the "oneeach" family that will be used in this example.
Figure 6: Plot of the `complete_sa` object. Nearest-neighbor positions have strong interactions (with negative potential) for different-valued pairs, while position (4, 4) has a weaker positive potential. This can be interpreted as nearest-neighbors having more weight when they are equal, while pixel with relative position (4, 4) have more weight when they are different.

For estimating the set interacting positions $R$, we use use a naive algorithm which consists of performing 300 steps of Stochastic Approximation considering a large set of candidate interacting positions (all positions with maximum norm less or equal 6, 84 positions total) and then select the positions which absolute value of the associated potential is higher than a threshold value. This is a strategy similar to the heuristic search algorithm from Gimel’farb (1996). Stochastic approximation was preferred over maximum pseudo-likelihood, for example, because it is computationally more suited for high-dimensional situations and we are not requiring a very accurate estimation at this point, so we can use a relatively lower number of steps.

The code below implements this naive interaction selection algorithm in a few lines using the tools available in `mrf2d` considering a threshold value of 0.10.

```r
R> # Define a large set of interacting positions
R> candidates <- mrfi(6, norm_type = "m")
R>
R> # Stochastic approximations for the candidate set
R> set.seed(1)
R> complete_sa <- fit_sa(field1, candidates, family = "oneeach",
+   gamma_seq = seq(from = 1, to = 0, length.out = 300),
+   cycles = 2, refresh_each = 301)
R>
R> plot(complete_sa)
```
Markov Random Fields on lattices

```r
# Threshold-based selection
thr_value <- 0.1
theta_vec <- smr_array(complete_sa$theta, "oneeach")
selected <- which(abs(theta_vec) > thr_value)

R1 <- candidates[selected]
R1
```

3 interacting positions.

```
rx  ry
1   0
0   1
4   4
```

Figure 7: Candidate positions for the interaction structure (left) and selected positions (right).

**Estimating \( \theta \)** Considering the parameter restriction family "onepar" and the selected interaction structure \( R = \{(1,0),(0,1),(4,4)\} \), we have a model with 3 free parameters. A 3-dimensional optimization problem is simple enough to be solved using the built-in pseudolikelihood optimization function. We also fit the model via Stochastic Approximation, now only considering the selected interaction structure, for comparison. The obtained results are compared with the `summary()` method for the `mrfout` class and presented below.

```r
pl <- fit_pl(field1, R1, family = "oneeach")
summary(pl)
```

Model adjusted via Pseudolikelihood
Image dimension: 150 150
2 colors, distributed as:

```
    0   1
11083 11417
```

Interactions for different-valued pairs:

```
Position| Value  Rel. Contribution
(1,0)| -0.993 1.000 ***
(0,1)| -1.021 0.995 ***
(4,4)|  0.183 0.735 **
```
R> sa <- fit_sa(field1, R1, family = "oneeach",
+   gamma_seq = seq(from = 1, to = 0, length.out = 300))
R> summary(sa)

Model adjusted via Stochastic Approximation
Image dimension: 150 150
2 colors, distributed as:
          0      1
11083    11417

Interactions for different-valued pairs:
Position| Value  Rel. Contribution
(1,0)|-0.964 | 1.000 ***
(0,1)|-0.983 | 0.987 ***
(4,4)| 0.183 | 0.756 ***

Evaluating the fitted model To evaluate how well the estimated parameters fit the data, we generate a new sample from the fitted model. Figure 8 shows the original image and the image simulated from the fitted model for comparison. The patterns created are visually very similar. Therefore the MRF model fitted successfully describes the characteristics of the data and is capable of synthesizing new images with the same texture pattern.

R> z_sim <- rmrf2d(dim(field1), R1, pl$theta)

Figure 8: Original data (left) and random field simulated from the fitted model (right).

4.2. Example 2: Image segmentation of a Hidden MRF with spatial fixed effect

Description The data available in the object hfield1 in the package will be used to illustrate the use of mrf2d for Gaussian mixtures driven by Hidden MRFs. It consists of an image
with continuous-valued pixels ranging from 0.3 to 15.2. A pattern similar to the previous example can be observed with the addition of a continuous noise.

```r
R> data("hfield1", package = "mrf2d")
R> cplot(hfield1)
```

![Figure 9: Image data for hfield1.](image)

We consider the image as a latent Hidden MRF and a random noise which the distribution on each pixel distribution depends its label. The main goal in this type of data is to recover the segmentation of the underlying pixel labels, as an image segmentation problem (Li, Wu, and Zhang 2009; Shah and Chauhan 2015, for example). This is the typical problem where Gaussian mixtures driven by hidden Markov random fields are suited for.

**Fitting a Hidden MRF with no fixed effect**  The built-in function for fitting Hidden MRFs (fit_ghm()), just like most algorithms used for Gaussian mixtures driven by HMRFs, considers the distribution of the underlying field as a hyper-parameter specified a priori. In this example, because a pattern similar to the one observed in the previous example can be seen forming two cluster of gray levels locally across the image, we will reuse the model fitted in Example 1 as the MRF distribution.

We fit a HMRF model to the data using the fit_ghm function. The mixture parameters estimates are below and the resulting segmentation is presented in Figure 10(b).

```r
R> hmrf_nofixed <- fit_ghm(hfield1, mrfi = R1, theta = pl$theta)
R> summary(hmrf_nofixed)
```

Gaussian mixture model driven by Hidden MRF fitted by EM-algorithm.

Image dimensions: 150 150

Predicted mixture component table:

|   | 0 | 1 |
|---|---|---|
| 0 | 11031 | 11469 |

Number of covariates (or basis functions): 0

Interaction structure considered: (1,0) (0,1) (4,4)
Mixture parameters:

| Component | mu   | sigma |
|-----------|------|-------|
| 0         | 5.30 | 1.40  |
| 1         | 9.20 | 1.46  |

Model fitted in 5 iterations.

The labels in the segmentation follow the expected pattern only in the middle part of the image. Two large clusters without the pattern appear at the upper and lower parts of the image, what indicates there might be some missing spatial information not included in the model.

**Adding a polynomial trend as fixed effect** A HMRF model without covariates has an intrinsic assumption that the mean values of pixel intensities given its labels are homogeneous along the image region. This is not the case for the considered data, as a vertical gradient effect can be observed.

In order to correct this spatial effect not captured in the model, we include spatial covariates, in form of polynomial functions of pixel positions \((i_1, i_2)\) as fixed effect. These covariates can be specified in `fixed_fn` argument of the function and a (centered) polynomial can be created with the `polynomial_2d()` function from `mrf2d`.

In this example, we include all terms of a two-dimensional centered polynomial which maximum degree of the components of its terms are 3, i.e.,

\[
p(i_1, i_2) = \sum_{d_1=0}^{3} \sum_{d_2=0}^{3} \beta_{i_1,i_2} (i_1 - c_1)^{d_1} (i_2 - c_2)^{d_2},
\]

where the centering position \((c_1, c_2)\) is the middle pixel position of the image.

R> hmrf_poly <- fit_ghm(hfield1, mrfi = R1, theta = pl$theta, + fixed_fn = polynomial_2d(c(3,3), dim(hfield1)))
R> summary(hmrf_poly)

Gaussian mixture model driven by Hidden MRF fitted by EM-algorithm.

Image dimensions: 150 150

Predicted mixture component table:

|   |     |     |
|---|-----|-----|
| 0 | 11559 | 10941 |

Number of covariates (or basis functions): 15

Interaction structure considered: (1,0) (0,1) (4,4)

Mixture parameters:

| Component | mu   | sigma |
|-----------|------|-------|
| 0         | 6.78 | 0.62  |
| 1         | 7.81 | 1.19  |

Model fitted in 5 iterations.
The code chunk below illustrates how the resulting fields available in the function output can be visualized. The results are presented in Figure 10.

```
R> cplot(hfield1)
R> dplot(hmrf_nofixed$Z_pred, legend = TRUE)
R> cplot(hmrf_poly$fixed)
R> dplot(hmrf_poly$Z_pred, legend = TRUE)
```

![Figure 10: Results from the Hidden MRF fits: (a) the original image data, (b) segmentation obtained without adding a polynomial effect, (c) polynomial fitted as a fixed effect, (d) image segmentation when the polynomial effect is included.](image)

This example highlights the two features of `mrf2d` that are not available in other packages: The possibility to specify a distribution for the underlying field that is more flexible than a simple Potts model and the option to include covariates (in this example, the polynomial trend) that are estimated in the simultaneously to the mixture parameters, allowing us to prevent undesired effects in the segmentation results.

### 4.3. Example 3: Neuroimaging segmentation with BOLD5000 data

Neuroimaging is one of the most frequent applications of HMRF models (Zhang et al. 2001; Shah and Chauhan 2015). We illustrate a brain magnetic resonance image segmentation using
a sample of the BOLD5000 dataset (Chang, Pyles, Marcus, Gupta, Tarr, and Aminoff 2019) available in the bold5000 object in the package.

\begin{verbatim}
R> data("bold5000", package = "mrf2d")
R> cplot(bold5000)
\end{verbatim}

\begin{figure}[h]
\centering
\includegraphics[width=\textwidth]{brain_image.png}
\caption{Brain magnetic resonance image in \texttt{bold5000} data.}
\end{figure}

Our main goal in this problem is to segment the brain image into large regions that corresponds to different elements, like a background, bones, fat, grey matter, white matter, etc.

The most common approach for the segmentation using HMRFs is to consider a simple Potts model (nearest-neighbor interaction structure $\mathcal{R} = \{(1, 0), (0, 1)\}$ and the "\texttt{onepar}" parameter restriction family. The potential associated with different-valued pairs controls, as well as the number of components are considered fixed a priori and will not be discussed in this paper. For the purpose of illustration, we use 4 components ($C = 3$) and the value $-1$ for the potentials of different-valued pairs.

\begin{verbatim}
R> Rnn <- mrfi(1)
R> theta_nn <- expand_array(-1, family = "onepar", C = 3, mrfi = Rnn)
R> theta_nn

, , (1,0)
 0 1 2 3
0 0 -1 -1 -1
1 -1 0 -1 -1
2 -1 -1 0 -1
3 -1 -1 -1 0

, , (0,1)
 0 1 2 3
0 0 -1 -1 -1
\end{verbatim}
We add a constraint that all variance parameters of the mixture components must be equal by setting the `equal_vars` parameter to `TRUE`. This improves the results in this problem by preventing some of the mixture components to be estimated with too high variance, what may causes pixels with values too high and too low to be predicted of the same class with high probability.

We also fit an independent Gaussian mixture (by multiplying all the to potentials by zero) for a comparison with the HMRF model. Segmentation results are presented in 12 and the parameter estimates are shown below.

```R
R> fit_brain <- fit_ghm(bold5000, Rnn, theta_nn, equal_vars = TRUE)
R> fit_brain_ind <- fit_ghm(bold5000, Rnn, theta_nn*0, equal_vars = TRUE)
```

```R
R> summary(fit_brain)
```

Gaussian mixture model driven by Hidden MRF fitted by EM-algorithm.
Image dimensions: 176 256
Predicted mixture component table:

|   | 0   | 1   | 2   | 3   |
|---|-----|-----|-----|-----|
| 22867 | 6813 | 7401 | 7975 |

Number of covariates (or basis functions): 0
Interaction structure considered: (1,0) (0,1)

Mixture parameters:

| Component | mu   | sigma |
|-----------|------|-------|
| 0         | 7.11 | 28.77 |
| 1         | 128.04 | 28.77 |
| 2         | 207.34 | 28.77 |
| 3         | 294.83 | 28.77 |

Model fitted in 14 iterations.

```R
R> summary(fit_brain_ind)
```

Gaussian mixture model driven by Hidden MRF fitted by EM-algorithm.
Image dimensions: 176 256
Predicted mixture component table:

|   | 0   | 1   | 2   | 3   |
|---|-----|-----|-----|-----|
| 23013 | 7020 | 7066 | 7957 |

Number of covariates (or basis functions): 0
Interaction structure considered: (1,0) (0,1)

Mixture parameters:
Component    mu    sigma
0    7.51    30.23
1    133.10    30.23
2    211.72    30.23
3    295.33    30.23

Model fitted in 4 iterations.

The resulting parameter estimates are not much different when comparing the independent mixture model and the HMRF, but the segmentation is cleaner when using the HMRF model, without sparse different-labeled pixels inside regions.

R> dplot(fit_brain$Z_pred, legend = TRUE)
R> dplot(fit_brain_ind$Z_pred, legend = TRUE)

Figure 12: Image segmentation predicted by the Hidden MRF fitted (left) and the independent mixture model (right).

5. Discussion

mrf2d provides a consistent programming interface for statistical inference in a large class of discrete Markov Random Field models defined on 2-dimensional lattices. It has an efficient and simple to use implementation of the main stack of computations used by most of inference algorithms, as well as complete routines for some commonly used and more complex estimation methods. The objects used for representing each model component have been carefully designed and tuned over several iterations to achieve a balance between performance and usability in the stable version.

The model featured in the package generalizes Potts model from other available packages in different ways, such as allowing a flexible definition of interacting pixel positions and interaction types, with the drawback that it cannot take advantage of algorithms that require the setup of a Potts model to improve their efficiency.
We currently have over 160 unit tests supported by the `testthat` package (Wickham 2011) and more than 90% of the code covered in the tests. These tests were designed to verify mathematical correctness of functions, the behavior of functions with unexpected input and the consistency of error messages. The package is in constant development and new tests are added whenever new functionalities are implemented to ensure its reliability over time.

For these reasons, `mrf2d` is another important tool for making statistical inference in images using Markov Random Fields more accessible, allowing researchers to produce data analysis and implement new algorithms in R with a simple and consistent framework.

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A. Customizing visualizations with ggplot2

A.1. Random Field Visualization

The two plotting functions `dplot()` and `cplot()` return an object of the `ggplot` class, what allows users to produce customized visualizations by changing scales, legend characteristics, titles, themes and much more by using the grammar of graphics from the `ggplot2` package (Wickham 2016).

Random fields (represented by `matrix` objects) are transformed into a `data.frame` structure with columns `x`, `y` and `value`. `x` and `y` are the indices of the matrix object while `value` maps the pixel-value in that position ($Z[x,y]$).

The plots are constructed using a tile plane with rectangles (`geom_tile()` from `ggplot2`) with the `value` column map to the `fill` aesthetics. In `dplot()`, which is used for finite-valued fields, `value` is treated as a factor, while in `cplot()` it is a continuous numeric. This is the only difference between the functions and it should be kept in mind when defining custom color scales.

Figure 13 created with the code chunk below shows examples of customized versions of a random field visualization built from the same base `dplot()` result. Modifications include adding a title, removing all scale-related information (keeping only the actual image), using a custom color-scale and changing the legend position, respectively.

```r
R> library("ggplot2")
R> base_plot <- dplot(field1, legend = TRUE)
R>
R> base_plot + ggtitle("This is a custom title")
R> base_plot + theme_void() + theme(legend.position = "none")
R> base_plot + scale_fill_manual(values = c("red", "blue"))
R> base_plot + theme(legend.position = "bottom")
```

A.2. Interaction Structure Visualization

Similarly to the functions used to visualize random fields, the `plot()` method for `mrfi` objects. A `data.frame` with columns named `rx` and `ry` is created internally with the coordinates of each interacting relative position. These columns are mapped to the `x` and `y` axis, respectively and a `geom_tile` is used to produce the plot. The reverse positions are included automatically with a light-gray color, but this can be prevented by setting `include_opposite = FALSE` in the `plot` call. It also returns a `ggplot` object that can be customized.

```r
R> mrfi_plot <- plot(mrfi(3) + c(5,1))
R>
R> # Custom colors
R> mrfi_plot + geom_tile(fill = "orange", color = "blue")
R> # Adding labels with `geom_text`
R> mrfi_plot + geom_text(aes(label = paste0("","rx","","ry","")))
R> # Custom title
```
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Figure 13: Four examples of field visualizations achieved by adding `ggplot2` layers to a base plot produced in `mrf2d`.

```r
R> mrfi_plot + ggtitle("Add a custom title") +
+   theme(plot.title = element_text(hjust = 0.5, size = 24))
```

Figure 14: Examples of customized visualizations of `mrfi` objects.
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