Discrete Markov Random Fields

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Binary MRFs on regular lattices

- Defined on a lattice $\mathbf{x} = \{x_1, \ldots, x_n\}$.
- Lattice points $x_i$ take values $\{-1, 1\}$.
- Full conditional $p(x_i|x_{-i}, \theta) = p(x_i|\text{neighbours of } i, \theta)$.

$$p(x|\theta) \propto q(x|\theta) = \exp \left\{ \theta_0 \sum_i x_i + \frac{1}{2} \theta_1 \sum_{i \sim j} x_i x_j \right\}.$$  

Here $\sim$ means "is a neighbour of".
Binary MRFs on regular lattices

The Markov property
Binary MRFs on regular lattices

The Markov property
The normalising constant is typically *difficult* to compute:

$$z(\theta) = \sum_{x_1} \cdots \sum_{x_n} q(x|\theta).$$
Our problem of interest

How can statistical inference be carried for a model

\[ p(x|\theta) = \frac{q(x|\theta)}{z(\theta)} , \]

where \( z(\theta) \) is an intractable normalising constant?
Maximum likelihood estimation:

\[ \hat{\theta} = \arg \max_\theta p(x|\theta) = \arg \max_\theta \frac{q(x|\theta)}{z(\theta)}. \]

Bayesian inference:

Here we use the posterior distribution \( p(\theta|x) \propto p(x|\theta)p(\theta) \).
A Metropolis-Hastings MCMC scheme requires calculation of

\[ \frac{p(x|\theta^*)p(\theta^*)}{p(x|\theta)p(\theta)} = \frac{q(x|\theta^*)p(\theta)}{q(x|\theta)p(\theta)} \frac{z(\theta)}{z(\theta^*)}. \]
Posterior distributions of the type

\[
p(\theta|\mathbf{x}) \propto p(\mathbf{x}|\theta)p(\theta) = \frac{q(\mathbf{x}|\theta)}{z(\theta)}p(\theta)
\]

are sometimes called doubly intractable distributions.

This type of complication occurs frequently for Markov random field models.
Posterior distributions of the type

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\[ = \frac{q(x|\theta)}{z(\theta)}p(\theta) \]

are sometimes called **doubly intractable** distributions.

This type of complication occurs frequently for *Markov random field* models.
Realisations of binary MRfs

As the parameter $\theta$ increases, the level of spatial aggregation does too.

Hidden MRFs

Here a true scene $x$ is corrupted by a noise process with parameters $\mu$ yielding data $y$. The aim to infer all unknown parameters.
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Hidden MRFs

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Standard MCMC algorithm

**Step 1. Update each** $x_i$ **in turn by Gibbs sampling from:**

$$p(x_i|x_{\setminus i}, y, \theta, \mu) \propto p(y_i|x_i, \mu)p(x_i|x_{N(i)}, \theta).$$ (1)

**Step 2. Update** $\mu$: **Carry out a M-H update of** $\mu$ **from the full conditional:**

$$p(\mu|x, y, \theta) \propto \left\{ \prod_{i=1}^{n} p(y_i|x_i, \mu) \right\} \pi(\mu).$$

**Step 3. Update** $\theta$: **Carry out a M-H update of** $\theta$ **from the full conditional:**

$$p(\theta|x, \mu, y) \propto p(x|\theta)\pi(\theta).$$
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$$p(\mu|x, y, \theta) \propto \left\{ \prod_{i=1}^{n} p(y_i|x_i, \mu) \right\} \pi_\mu(\mu).$$

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$$p(\theta|x, \mu, y) \propto p(x|\theta)\pi_\theta(\theta).$$
We now concentrate on how to deal with the intractable normalising constant $z(\theta)$.
Undirected Graphs and joint distributions

The joint distribution can be written as

$$p(x_1, \ldots, x_6) = \frac{1}{z} \psi(x_1, x_2) \psi(x_1, x_3) \psi(x_2, x_4) \psi(x_3, x_6) \psi(x_2, x_5, x_6).$$

Naively, the normalising constant is computed as

$$z = \sum_{x_1} \cdots \sum_{x_6} \psi(x_1, x_2) \psi(x_1, x_3) \psi(x_2, x_4) \psi(x_3, x_6) \psi(x_2, x_5, x_6).$$

Computational complexity scales as $s^6$ (assuming $x_i$ has $s$ states).
Undirected Graphs and joint distributions

However,

\[ z = \sum_{x_1} \sum_{x_2} \psi(x_1, x_2) \sum_{x_3} \psi(x_1, x_3) \sum_{x_4} \psi(x_2, x_4) \]

\[ \sum_{x_6} \psi(x_3, x_6) \sum_{x_5} \psi(x_2, x_5, x_6) . \]

No more than 3 terms appear in any summand. Computational complexity is decreased!

In general we would like to perform the summation so that the largest factor is as small as possible.
MRF in factorisable form

Define an index \( i = 1, \ldots, n \), where points are ordered from top to bottom and rows from left to right. \( m \) denotes the number of rows.

\[
q(x|\theta) = q_n(x_n|\theta) \prod_{i=1}^{n-1} q_i(x_i|x_{i+1:n}, \theta),
\]

where we define

\[
q_i(x_i|x_{i+1:n}, \theta) = \exp(\theta_0 x_i + \theta_1 x_i (x_{i+1} + x_{m+i}))
\]

with modifications when \( i \) corresponds to a point on the last row or column.
MRF in factorisable form

We use the shorthand notation $x_{i:j} = (x_i, \ldots, x_j)$.

$$z(\theta) = \sum_{x_1} \sum_{x_2} \cdots \sum_{x_n} q_1(x_1|x_2:n, \theta)q_2(x_2|x_3:n, \theta) \cdots q_n(x_n|\theta)$$

$$= \sum_{x_1} q_1(x_1|x_2:n, \theta) \sum_{x_2} q_2(x_2|x_3:n, \theta) \cdots \sum_{x_n} q_n(x_n|\theta).$$
The recursive algorithm
Reeves and Pettitt, Biometrika (2004)

\[
\begin{align*}
z_1(\theta, x_{2:n}) &= \sum_{x_1} q_1(x_{1:m+1}, \theta) \\
z_i(\theta, x_{i+1:n}) &= \sum_{x_i} q_i(x_{i:m+i}, \theta) z_{i-1}(\theta, x_{i:n}), \text{ for } i = 2, \ldots, n. \\
z(\theta) &= z_n(\theta)
\end{align*}
\]
Exact sampling: The recursive algorithm

NF and Rue, Biometrika (2007)

\[
\begin{align*}
  z_1(\theta, x_{2:n}) &= \sum_{x_1} q_1(x_{1:m+1}, \theta) \\
  z_i(\theta, x_{i+1:n}) &= \sum_{x_i} q_i(x_{i:m+i}, \theta)z_{i-1}(\theta, x_{i:n}), \text{ for } i = 2, \ldots, n.
\end{align*}
\]

Effectively \( z_i \) is the normalising constant for

\[
p(x_{1:i}|x_{i+1:n}, \theta) \propto q(x_{1:i}|x_{i+1:n}, \theta)
\]

Each \( z_i \) depends on \( m \) variables \( x_{i+1:m+1} \) - In total there are \( 2^m \)!
Exact sampling: The recursive algorithm

\[ p(x|\theta) = p(x_1|x_2:n, \theta)p(x_2|x_3:n, \theta) \ldots p(x_n|\theta). \]

We gather a sample from \( p(x|\theta) \) by sampling from

\[
p(x_i|x_{i+1:n}, \theta) = \frac{p(x_{1:i}|x_{i+1:n}, \theta)}{p(x_{1:i-1}|x_{i:n}, \theta)} = \frac{q(x_{1:i}|x_{i+1:n}, \theta)z_{i-1}(\theta, x_{i:n})}{q(x_{1:i-1}|x_{i:n}, \theta)z_i(\theta, x_{i+1:n})},
\]

for \( i = n, n-1, \ldots, 1. \)
Exact sampling: The recursive algorithm

We propose a two pass algorithm:

**Forwards pass:** Using the recursive scheme above, we generate in turn each $z_i(\theta, x_{i+1:n})$ for $i = 1, 2, \ldots, n$.

**Backwards pass:** Sample $x_i$ from $p(x_i|x_{i+1:n}, \theta)$ using the $z_i$’s, for $i = n, n - 1, \ldots, 1$. 
Computer implementation

- Main computational loads arises from generating the collection of $z_i$’s from the forwards pass. For each $z_i$, there are $2^m$ realisations, in total $n \times 2^m$.
- In our computer implementation, we can sample lattices where the smaller dimension is $\leq 19$. For example, a $19 \times 19$ lattice takes about 150 seconds.
Extensions of the algorithm

The algorithm can be extended to:

1. sample from $p(x|\theta)$.
2. sample from $p(x|\theta, y)$, where $y$ is a hidden version of $x$.
3. compute the modal lattice for $p(x|\theta, y)$. Again a two pass algorithm is used, essentially sampling from an annealed distribution at temperature 0.
4. compute the marginal distribution of points, pairs of points, eg $p(x_i|\theta)$, $p(x_i, x_j|\theta, y)$ for neighbours $i, j$.
5. different neighbourhood structures.
6. more than 2 states.

Details appear in (Friel & Rue, Biometrika, 2007)
Further extensions: hidden MRFs

Consider the posterior marginal for $\theta$. For any realisation $x$,

$$p(\theta|y) = \frac{p(x, \theta|y)}{p(x|\theta, y)}.$$

We can write this as

$$p(\theta|y) \propto \frac{p(y|x)p(x|\theta)p(\theta)}{p(x|\theta, y)},$$

the normalising constant is $p(y)$ - the marginal likelihood.

Each term on the RHS above can be calculated exactly.

We estimate $p(\theta|y)$ and $p(y)$ by integrating (numerically) the RHS wrt $\theta$.

We estimate these marginals without using MCMC.
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Illustrative example - moderately sized lattice

Data consist of measurements of soil phosphate content on a $16 \times 16$ grid at 10 metre intervals at a location in northern Greece (Besag, York, Mollie, 1989).

Model $k = 1$: MRF where each point has 4 nearest neighbours.  
Model $k = 2$: MRF where each point has 8 nearest neighbours.

We assume $y$’s are conditionally independent given $x$’s with normal distribution with known means and unknown common variance $\kappa$. 
Illustrative example - moderately sized lattice

\[ p(\theta, \kappa|y, k = 1) \quad \text{\&} \quad p(\theta, \kappa|y, k = 2) \]

Marginal likelihoods:

\[ \log p(y|k = 1) = -110.168 \quad \text{\&} \quad \log p(y|k = 2) = -114.075 \]

Assuming equally weighted models, a priori, yields

\[ p(k = 1|y) = 0.98 \quad \text{\&} \quad p(k = 2|y) = 0.02 \]
Now we ask how we can use the exact results on small lattices to do approximate inference for larger lattices.
Large lattice approximation

Strategy: Utilise exact results on sub-lattices.

\[ p(x|\theta) = p(x_A|\theta, x_c) p(x_c|\theta) p(x_B|\theta, x_c). \]

Assume we can compute both \( p(x_A|\theta, x_c) \) and \( p(x_B|\theta, x_c) \).

The problem remains to compute \( p(x_c|\theta) \).
Consider a sub-lattice, $x^* = x_S \cup x_c \cup x_T$.

$$p(x_c|\theta) = \frac{p(x|\theta)}{p(x_A|x_c, \theta)p(x_B|x_c, \theta)} 
\approx \frac{p(x^*|\theta)}{p(x_S|x_c, \theta)p(x_T|x_c, \theta)}.$$
Large lattice approximation

Consider a sub-lattice, \( x^* = x_S \cup x_c \cup x_T \).

\[
p(x_c | \theta) = \frac{p(x | \theta)}{p(x_A | x_c, \theta)p(x_B | x_c, \theta)} \approx \frac{p(x^* | \theta)}{p(x_S | x_c, \theta)p(x_T | x_c, \theta)}.
\]
Large lattice approximation

Performance of the approximation

- A $19 \times 19$ realisation from an Ising model with $\theta = 0.4$ was sampled. Gaussian noise with zero mean and unit variance was added to each state value leaving data $y$.
- We can compute $p(\theta|y)$ very precisely, since we can compute $p(x|\theta)$ and $p(x|\theta, y)$ exactly.
- We can compare this to an estimate of $p(\theta|y)$ using the approximations to $p(x|\theta)$ and $p(x|\theta, y)$ by covering the middle column with a sub-lattice of size $19 \times 5$. 
Illustrative example - larger sized lattice

Gene expressions were measured across the whole genome of *Plasmodium falciparum*, the organism that causes human malaria, for 46 1-hour consecutive intervals.

This example focuses on the relatively short mitochondrial chromosome, which consists of 72 genes and about which relatively little is known.

The data $y$ is observed on a $46 \times 72$ spatial-temporal rectangular lattice. $y_{tg}$ is the log-expression of gene $g$ at time $t$. 
Illustrative example - larger sized lattice

Latent model

The latent process is modelled a non-homogeneous Ising distribution with 2 states \{-1, 1\} corresponding to ‘up-regulation’ and ‘down-regulation’.

\[
p(x|\theta) \propto \exp (\theta_t V_t(x) + \theta_g V_g(x)).
\]

- \(V_t(x)\) measures the interactions between neighbouring lattice points corresponding to the same gene in the ‘time’ direction.
- \(V_g(x)\) similarly measures interactions at the same time point between neighbouring genes.
Illustrative example - larger sized lattice

Large lattice approximation

- The $46 \times 72$ lattice was partitioned into 3 disjoint sub-lattices of dimension $46 \times 17$ and a final sub-lattice of dimension $46 \times 18$, each separated by a column of lattice points.

- To compute the marginal distribution of the columns of lattice points, a lattice of size $17 \times 46$ was used to cover each column.
Illustrative example - larger sized lattice

Results

\[ p(\theta_t | y) \quad p(\theta_g | y) \]
We now focus on some further approaches to approximate $p(x|\theta)$ for large lattices $x$. 
Alternative large lattice approximations

Reduced dependence approximations (RDA)

Let \( r_i \) denote the \( i \)th row vector.

\[
\pi(x|\theta) = \pi(r_m|\theta) \prod_{i=1}^{m-1} \pi(r_i|r_{i+1:m}, \theta).
\]

We estimate each term on the RHS by conditioning on a reduced number of rows \( m_1 \).

\[
\pi(x|\theta) \approx \pi(r_{m-m_1+1:m}|\theta) \prod_{i=1}^{m-m_1} \pi(r_i|r_{i+1:i+m_1}, \theta).
\]

Each factor is further approximated as

\[
\pi(r_i|r_{i+1:i+m_1}, \theta) \approx \frac{\pi(r_{i:i+m_1}|\theta)}{\pi(r_{i+1:i+m_1}|\theta)}.
\]
Alternative large lattice approximations

Reduced dependence approximations (RDA)

\[
\pi(r_i | r_{i+1:i+m_1}, \theta) \approx \frac{\pi(r_{i:i+m_1} | \theta)}{\pi(r_{i+1:i+m_1} | \theta)}.
\]

Note that each probability appearing above can be calculated using the recursion method, provided \( m_1 \leq 20 \). In fact,

\[
\pi(x | \theta) \approx \frac{q(x | \theta)}{(z_{m_1}(\theta))^{m-m_1+1}/(z_{m_1-1}(\theta))^{m-m_1}}.
\]

Effectively, we approximate the overall NC as

\[
z(\theta) = \frac{(z_{m_1}(\theta))^{m-m_1+1}}{(z_{m_1-1}(\theta))^{m-m_1}}.
\]
Alternative large lattice approximations

Reduced dependence approximations (RDA)

What does this approximation depend on?

- The size of $m_1$ - the closer to $m$ the better.
- The value of $\theta$ - the closer to 0 the better.

This plot displays approximations to the log NC for a $50 \times 50$ lattice with $\theta = [0, 0.4]$ for values of $m_1 = 3, \ldots, 16.$
Alternative large lattice approximations

Reduced dependence approximations (RDA)

We can compute the NC (quite fast) and exactly for a $16 \times 16$ lattice:

Here we investigate how close the approximate log NC is to the true log NC for different values of $m_1$

\[
\text{Ratio} \frac{\text{True}}{\text{Approx}} = 0.995 \text{ for } m_1 = 8
\]
Alternative large lattice approximations

Reduced dependence approximations (RDA)

- This NC approximation was used in MCMC estimation of hidden Markov random field and gave good performance even when the noise distribution and the level of spatial aggregation in the hidden field were strong.
- RDA has been applied in a variational setting by McGrory et al. *Statistics and Computing* (2009).
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Alternative large lattice approximations

Partially ordered Markov model defined on sub-lattices

POMMs are a generalisation of a Markov chain to a directed acyclic graph.

\[ \pi(x_{ij} | x_{-ij}, \theta) = \pi(x_{ij} | x_{i+1,j}, x_{i,j+1}, \theta) \]

Now the likelihood is tractable:

\[ \pi(x | \theta) = \prod_{i=1}^{n} \pi(x_{ij} | x_{i+1,j}, x_{i,j+1}, \theta) \]
Alternative large lattice approximations

Partially ordered Markov model defined on sub-lattices

Alternatively, we can write the likelihood as:

\[
\pi(x|\theta) = \left[ \prod_{i \in L_0} \pi(x_i) \right] \left[ \prod_{j=1}^{L} \prod_{i \in L_j} \pi(x_i|pa(x_i)) \right]
\]

Now suppose that each lattice point is a sublattice for which we can compute a likelihood...
Alternative large lattice approximations
Partially ordered Markov model defined on sub-lattices

Suppose lattice \( x \) is divided into \( L \) non-overlapping sublattices \( x_l \).

\[
\pi(x_l|\theta) = \frac{1}{z_l(\theta)} \exp(\theta_0 V_0(x_l) + \theta_f V_f(x_l))
\]

Naively we could assume independent sub-lattices,

\[
\pi(x|\theta) \approx \prod_{i=1}^{L} \frac{1}{z_l(\theta)} \exp(\theta_0 V_0(x_l) + \theta_f V_f(x_l))
\]

But now dependencies across boundaries of \( x_l \)'s have been ignored. We re-introduce these dependencies by defining a POMM with sublattices \( x_l \) as the nodes!
Alternative large lattice approximations

Partially ordered Markov model defined on sub-lattices

Now each sublattice $x_i$ is dependent on its parent sub-lattices:

$$\pi(x_i|\text{pa}(x_i), \theta) = \frac{1}{z_l(\theta, \text{pa}(x_i))} \exp(\theta_0 V_0(x_i) + \theta_f V_f(x_i) + \theta_f V_{pa}(x_i, \text{pa}(x_i)))$$

The interactions between $x_i$ and it’s two predecessors is taken care of by $V_{pa}(x_i, \text{pa}(x_i))$.

Note that the NC $z_l(\theta, \text{pa}(x_i))$ is now a function of the parent sublattices.

Likelihood now looks like:

$$\pi(x|\theta) \approx \pi(x_L) \prod_{l=1}^{L-1} \pi(x_l|\text{pa}(x_l))$$
Alternative large lattice approximations

Cylinder approximation – Pettitt, NF, Reeves, JRSSB (2003)

Assume the lattice is wrapped on a cylinder

Why is this useful?

Now every column has two neighbouring columns. Therefore, the distribution of the rows is stationary.

\[ p(x) = p(c_1, \ldots, c_n) = p(c_i, c_{i+1}, \ldots, c_n, c_1, \ldots, c_{i-1}), \]

where \( c_i \) is the vector of lattice points for column \( i \).
Alternative large lattice approximations

Cylinder approximation
Let the set of all possible values of $c_j$ be denoted by

$$A = \{a_1, \ldots, a_n\}, \text{where } N = 2^m.$$  

Theorem

*Suppose the unnormalised $q(x|\theta)$ can be factorised as*

$$q(x|\theta) = \prod_{i=1}^{n} h(c_j, c_j - 1)$$

*for a given positive real function $h(\cdot, \cdot)$ defined on $A \times A$. Then the normalising constant for $q(x|\theta)$ is given by $tr(Q^n)$ where $Q$ is an $N \times N$ matrix whose $k$th row $(Q_{k1}, \ldots, Q_{kn})$ is defined by*

$$h(c_1 = a_1, c_0 = a_k), h(c_1 = a_2, c_0 = a_k), \ldots, h(c_1 = a_N, c_0 = a_k)$$
Alternative large lattice approximations

Cylinder approximation

Some remarks:

1. $Q$ is almost like a transition probability matrix. (The $k$th row of $Q$ gives the probability to transition from $c_k = a_k$ to any other column).

2. 

$$h(c_1 = c_0) = \exp \left\{ \theta_0 \sum_{i=1}^{m} x_i + \theta_1 \sum_{i=1}^{m-1} x_{i1}x_{i+1,1} + \theta_1 \sum_{i=1}^{m} x_{i0}x_{i1} \right\}$$

The second term is the 'within' $c_1$ interactions, third term is the between $c_0, c_1$ interactions.

3. For a binary MRF, $Q$ is a $2^m \times 2^m$ matrix ($m = \text{no. of rows}$).

$$z(\theta) = tr(Q^n) = tr(D^n),$$

where $D$ is the matrix of eigenvalues of $Q$. 
Other approaches to handle intractable NCs

Recall: We are interested in the posterior

\[ p(\theta|x) \propto p(x|\theta)p(\theta) \]

where

\[ p(x|\theta) = \frac{q(x|\theta)}{z(\theta)}, \]

where \( z(\theta) \) is an intractable normalising constant.

**Approximate Bayesian Computation**

First, rejection sampling:

1. \( \theta \sim p(\theta) \).
2. Accept \( \theta \) with probability \( p(x|\theta) \).

Obviously step 2 is a problem.
Approximate Bayesian Computation

However... it is often relatively easy to simulate from the model.

1. \( \theta \sim p(\theta) \).
2. Simulate pseudo-data \( x^* \sim p(\cdot|\theta) \).
3. Accept \( \theta \) if \( s(x^*) = s(x) \), where \( s(\cdot) \) is sufficient for \( p(\cdot|\theta) \).

The target distribution in this case is

\[
p(\theta, x^*|x) \propto p(x|\theta)p(\theta)I[s(x^*) = s(x)]
\]

The rejection ratio is

\[
\frac{p(x|\theta)p(\theta)I[s(x^*) = s(x)]}{p(x^*|\theta)p(\theta)} = I[s(x^*) = s(x)]
\]

Notice that it doesn’t require calculation of \( p(x|\theta) \).

ABC is sometimes called *likelihood-free inference*.
Approximate Bayesian Computation

ABC comes with a caveat.

Simulating pseudo-data $x^*$ which is similar to $x$ can be difficult. Finding a sufficient statistics can also be a problem.

The ABC algorithm can be extended to augment the target even further...

$$p(\theta, x^*, \epsilon | x) \propto p(x|\theta)p(\theta)I[d(x^*, x) < \epsilon].$$

This relaxes the need for $x^*$ to be ‘identical’ to $x$. 
Other approaches

Thermodynamic integration

\[ \frac{z(\theta')}{z(\theta)} = \int_{\theta}^{\theta'} \mathbf{E} \log q(x|\theta^*) \, d\theta^* \]

Variational approximations

The variational approach is to propose a simple structural form for the approximation, \( q(x|\theta) \).

\[ \hat{\theta} = \arg \min_{\theta} KL [p(x|\theta) \parallel q(x|\theta)] \]

Sequential Monte Carlo

The sequential Monte Carlo approach of (Del Moral et al., 2006) should be useful in these contexts also.
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