An approximation for binary Markov random fields

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Introduction

- Binary (hidden) Markov random field

$$\pi(x|\theta) = \frac{1}{b(\theta)} \exp\left\{ - \sum_{C \in \mathcal{C}} V_C(x_C|\theta) \right\}$$

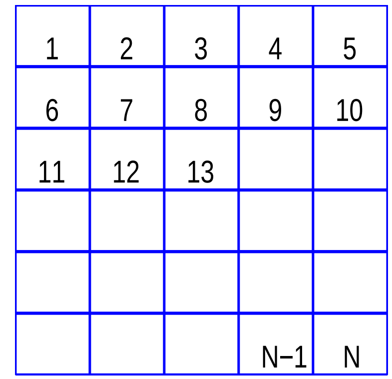
  - ex: Ising model (with external field)
- Likelihood evaluation not possible (MLE via MCMCMLE)
- Direct simulation not possible (simulation possible by MCMC)
- Our goals:
  - define approximate normalising constant
  - define approximate model from which direct simulation is possible
- Starting point: forward-backward recursion for MRF

Plan

- Notation
- Exact forward-backward recursion
- Approximate forward-backward recursion
- Evaluation criteria for approximation
  - compare to exact results (for small lattices)
  - compare results for different approximation levels
  - use approximation as proposal in independent proposal Metropolis–Hastings algorithm
- Simulation examples.

Notation

- Binary Markov random field on $n_I \times n_J$ lattice, $N = n_I \cdot n_J$
- State vector $x = (x_1, \ldots, x_N)$, with $x_i \in \{0, 1\}$



- Set of cliques: $\mathcal{C}$
- Joint distribution

$$\pi(x|\theta) = \frac{a(x|\theta)}{b(\theta)} \propto a(x|\theta) = \exp\left\{ -\sum_{C \in \mathcal{C}} V_C(x_C, \theta) \right\} = \prod_{C \in \mathcal{C}} e^{-V_C(x_C, \theta)}$$

- Reformulation

$$a(x|\theta) = \prod_{k=1}^{N} a_k(x_{k:k+p+1}, \theta)$$

  - p is a function of n_J and the clique size
  - for first-order pairwise interaction model: $p = n_J$

Exact forward recursion

- Following Pettitt and Reeves (2004) and Friel and Rue (2007)
- For illustration: Small 6×5 lattice, Ising model

$$\pi(x_{1:30}|\theta) = b(\theta)^{-1} a_1(x_{1:6}, \theta) a_2(x_{2:7}, \theta) a_3(x_{3:8}, \theta) \cdots$$

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&= b(\theta)^{-1} b_2(x_{2:6}, \theta) a_2(x_{2:7}, \theta) a_3(x_{3:8}, \theta) \cdots
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$$\pi(x_2|x_{2:30}, \theta) \propto b_2(x_{2:6}, \theta) a_2(x_{2:7}, \theta)$$

$$\pi(x_1|x_{2:30}, \theta) \propto b_1(x_{1:5}, \theta) a_1(x_{1:6}, \theta)$$

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- Computational complexity: forward: $O(N2^p)$, backward: cheap

Approximate forward recursion

- For illustration: Small 6×5 lattice, Ising model

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Approximate backward recursion

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Representation of $b_k(x_{k:k+p}, \theta)$

- Exact recursive formula

$$b_{k+1}(x_{k+1:k+p+1}, \theta) = \sum_{x_k} b_k(x_{k:k+p}, \theta) a_k(x_{k:k+p+1}, \theta)$$

- Number of values to store for each k: 2^p
- Represent $b_k(x_{k:k+p}, \theta)$ as

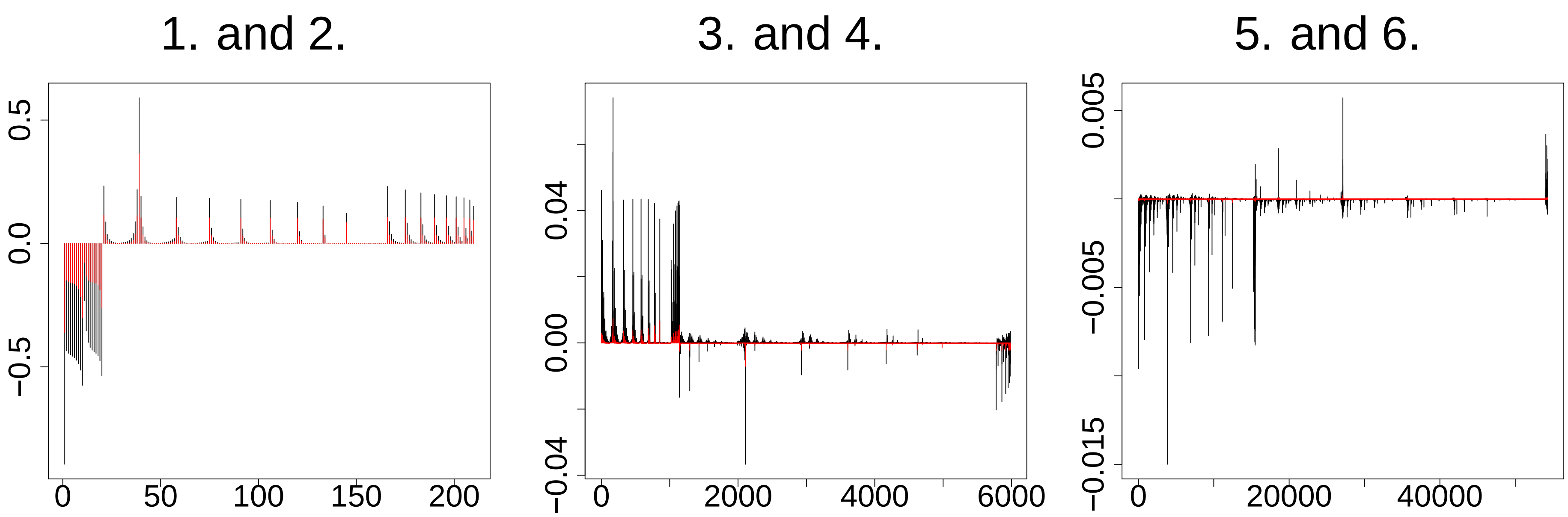
$$\ln\{b_k(x_{k:k+p}, \theta)\} = \beta_k^{\emptyset} + \sum_{i=k}^{k+p} \beta_k^{\{i\}} x_i + \sum_{i=k}^{k+p-1} \sum_{j=i+1}^{k+p} \beta_k^{\{i,j\}} x_i x_j$$

$$+ \sum_{i=k}^{k+p-2} \sum_{j=i+1}^{k+p-1} \sum_{t=j+1}^{k+p} \beta_k^{\{i,j,t\}} x_i x_j x_t + \ldots + \beta_k^{\{k,\ldots,k+p\}} x_k \cdot \ldots \cdot x_{k+p}$$

$$= \sum_{\Lambda \subseteq \{k,\ldots,k+p\}} \beta_k^{\Lambda} \prod_{i \in \Lambda} x_i$$

Ising example

- Ising model — small 20×20 lattice, i.e. $p = 20$
  - red: $\beta = 0.6$
  - black: $\beta = 0.8$



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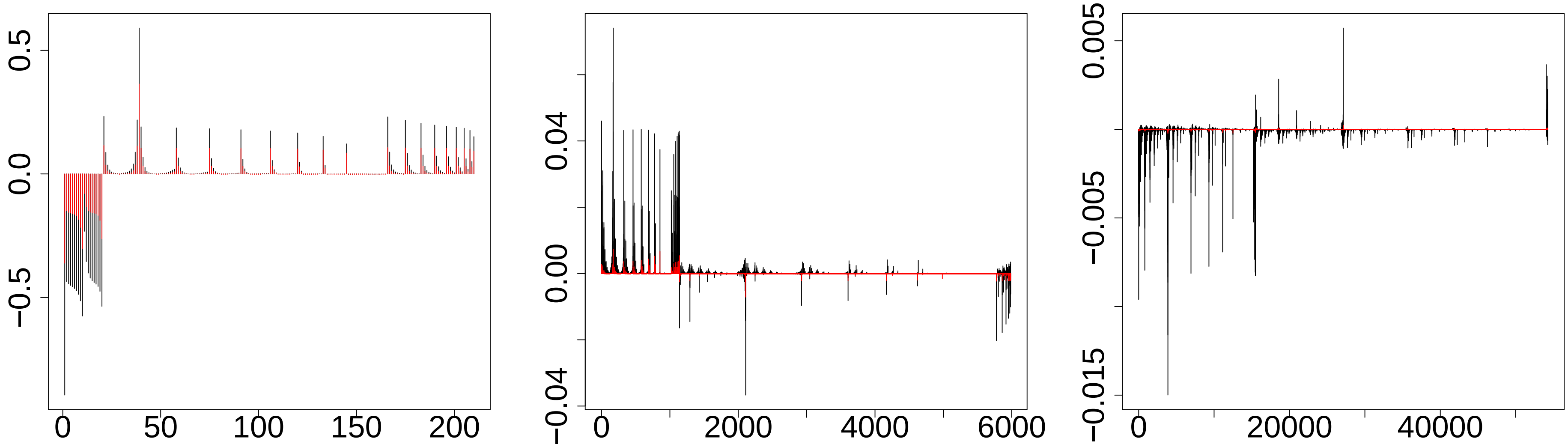
1. and 2.   3. and 4.   5. and 6.



- $\beta = 0.8$: fraction of interactions larger than ε

ε	10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}
fraction	0.000039	0.000169	0.000906	0.00556	0.0314

Forward recursion for new representation

- Correspondingly we represent

$$\ln\{a_k(x_{k:k+p+1},\theta)\} = \sum_{\Lambda\subseteq\{k,\ldots,k+p+1\}} \alpha_k^\Lambda \prod_{i\in\Lambda} x_i$$

- Old recursion formula

$$b_{k+1}(x_{k+1:k+p+1},\theta) = \sum_{x_k} b_k(x_{k:k+p},\theta)a_k(x_{k:k+p+1},\theta)$$

- Recursion formula for new representation

$$\exp\left\{\sum_{\Lambda\subseteq\{k+1,\ldots,k+p+1\}} \beta_{k+1}^\Lambda \prod_{i\in\Lambda} x_i\right\}$$
$$= \sum_{x_k} \exp\left\{\sum_{\Lambda\subseteq\{k,\ldots,k+p\}} \beta_k^\Lambda \prod_{i\in\Lambda} x_i + \sum_{\Lambda\subseteq\{k,\ldots,k+p+1\}} \alpha_k^\Lambda \prod_{i\in\Lambda} x_i\right\}$$

Recursive computation of β_{k+1}^{Λ}

- Setting $x_{k+1} = \ldots = x_{k+p+1} = 0$ gives

$$\exp\left\{\beta_{k+1}^{\emptyset}\right\} = \exp\left\{\beta_k^{\emptyset} + \alpha_k^{\emptyset}\right\} + \exp\left\{\beta_k^{\emptyset} + \beta_k^{\{k\}} + \alpha_k^{\emptyset} + \alpha_k^{\{k\}}\right\}$$

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- Setting $x_i = 1$ and $x_j = 0$ for all $j \neq i$ gives

$$\exp\left\{\beta_{k+1}^{\emptyset} + \beta_{k+1}^{\{i\}}\right\} = \exp\left\{\beta_k^{\emptyset} + \beta_k^{\{i\}} + \alpha_k^{\emptyset} + \alpha_k^{\{i\}}\right\}$$

$$+ \exp\left\{\beta_k^{\emptyset} + \beta_k^{\{i\}} + \beta_k^{\{k\}} + \beta_k^{\{k,i\}} + \alpha_k^{\emptyset} + \alpha_k^{\{i\}} + \alpha_k^{\{k\}} + \alpha_k^{\{k,i\}}$$

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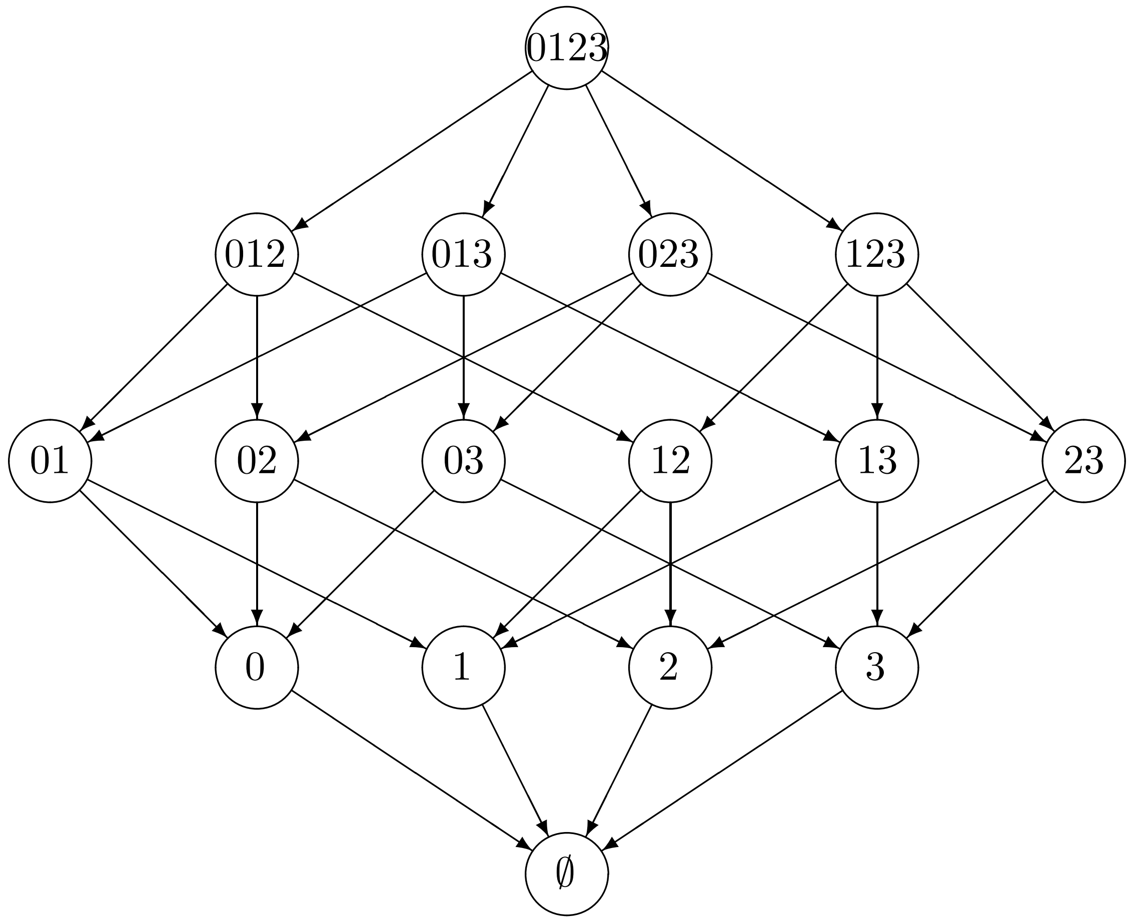
- Setting $x_i = x_j = 1$ and $x_t = 0$ for $t \notin \{i, j\}$ gives

$$\exp\left\{\beta_{k+1}^{\emptyset} + \beta_{k+1}^{\{i\}} + \beta_{k+1}^{\{j\}} + \beta_{k+1}^{\{i,j\}}\right\} = \ldots$$

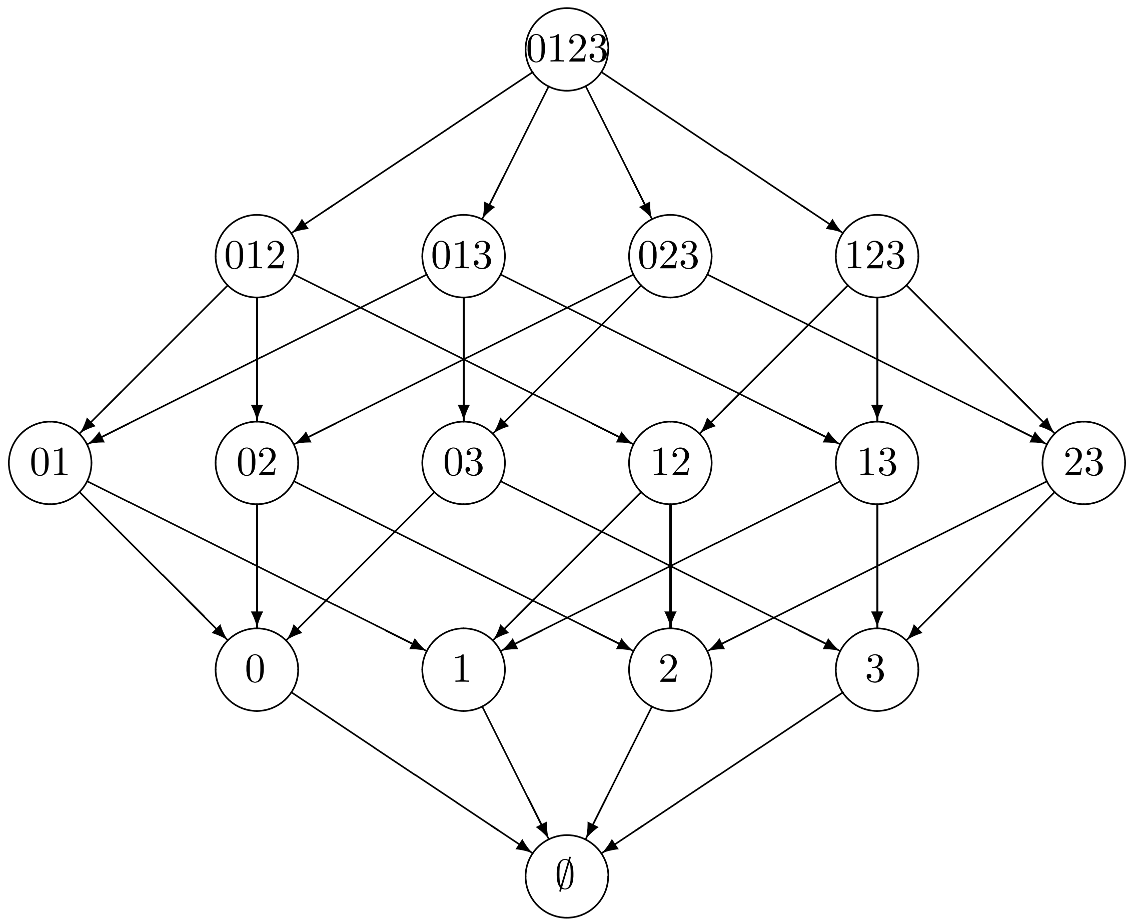
Recursive scheme

$$\ln\left\{b_k(x_{k:k+p},\theta)\right\} = \sum_{\Lambda\subseteq\{k,\ldots,k+p\}} \beta_k^{\Lambda} \prod_{i\in\Lambda} x_i$$



Approximation strategy

- If a computed β_k^Λ has $|\beta_k^\Lambda| \leq \varepsilon$, approximate β_k^Λ to zero
- If for some Λ, β_k^λ is (approximated to) zero for all $\lambda \subset \Lambda$, $|\lambda| = |\Lambda| - 1$, approximate β_k^Λ to zero (without computing the exact value)



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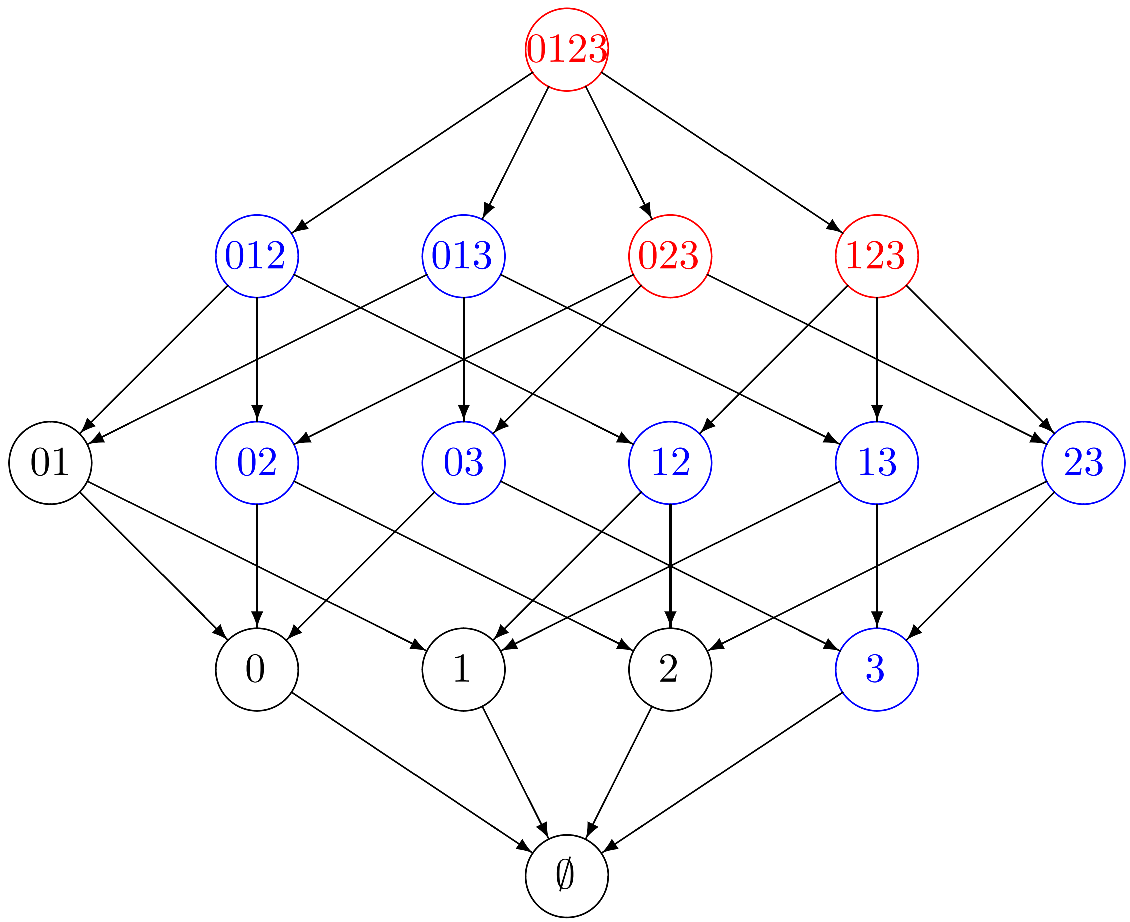


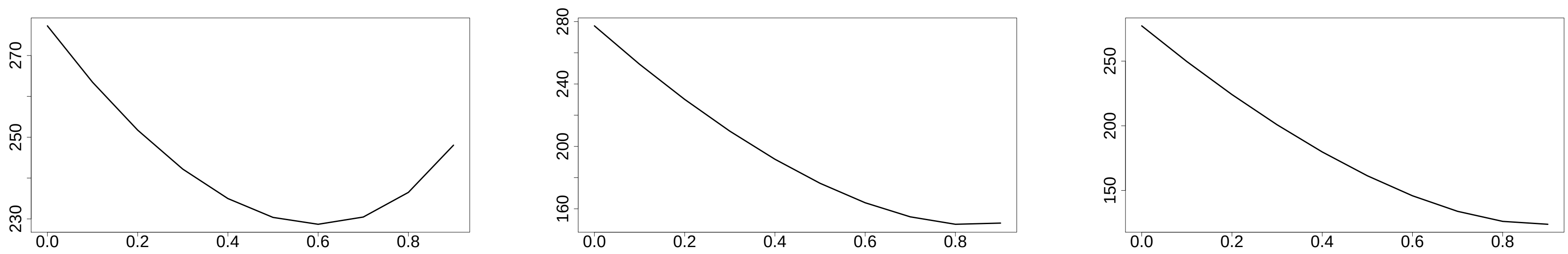
Evaluation criteria for approximation

- Compare approximation with exact result — for small lattices
- Compare results for different cut off values ε
- Use approximation as proposal in an independent proposal Metropolis–Hastings algorithm — look at acceptance rate

Comparison to exact results in a small lattice

- Ising model, small 20×20 lattice
- Simulate first a realisation from the Ising model
- Compute the likelihood function $l(\beta)$for this realisation
- Results for $\varepsilon = 0$, 10^{-5}, 10^{-4}, 10^{-3}, 10^{-2} and 10^{-1}

$\beta = 0.6$ $\beta = 0.8$ $\beta = 0.9$



Comparison to exact results in a small lattice

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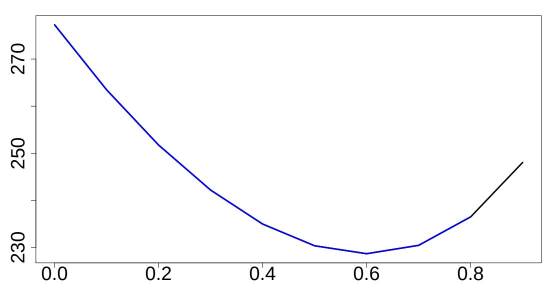

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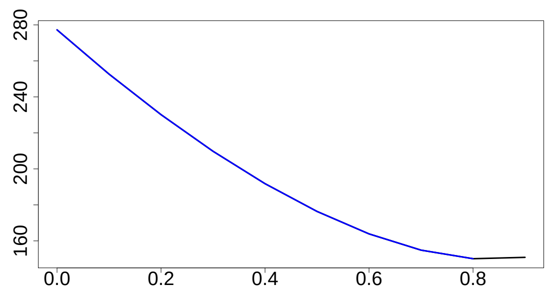

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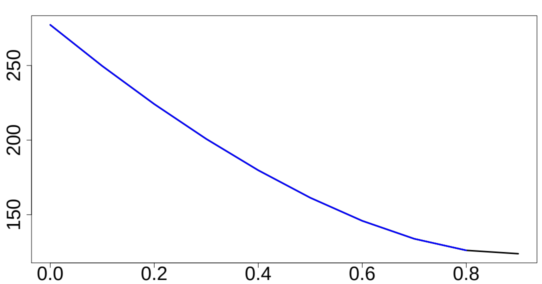

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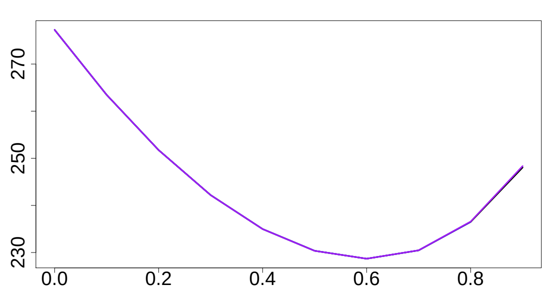

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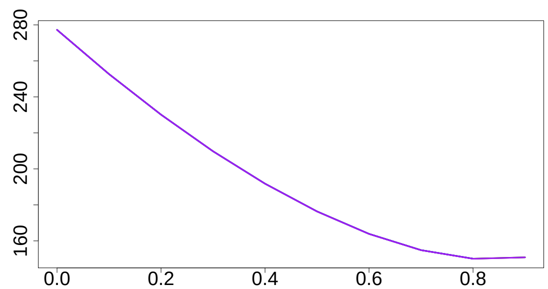

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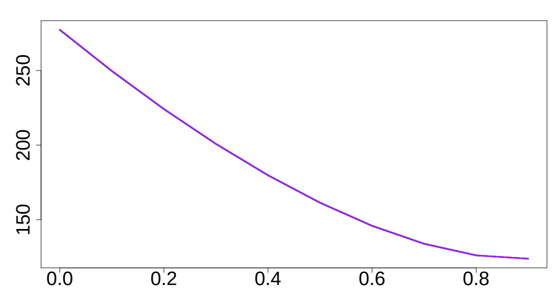

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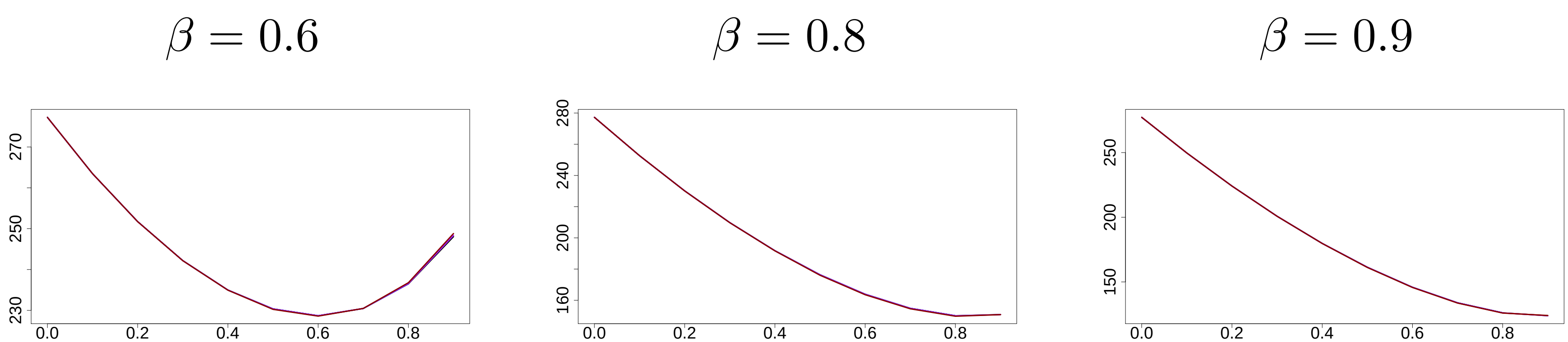

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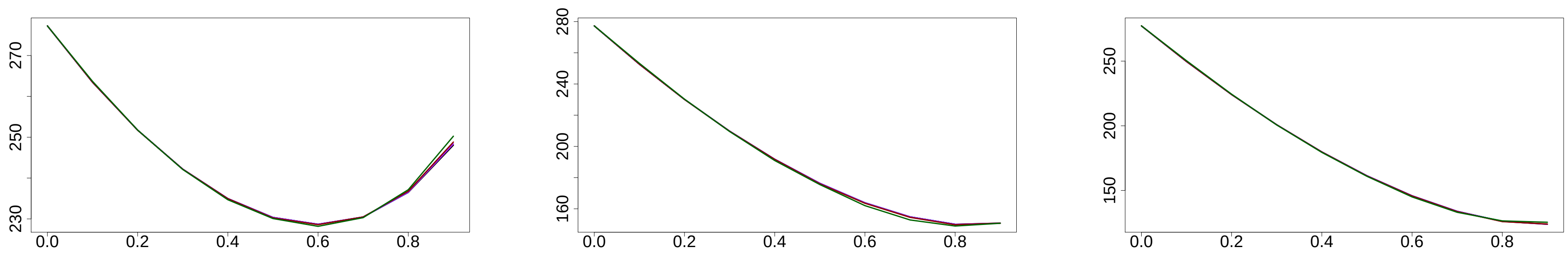

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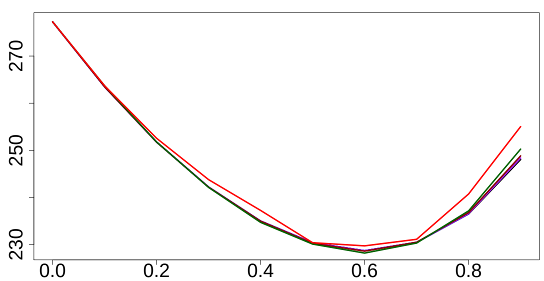

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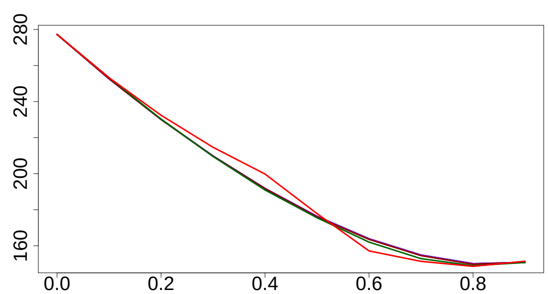

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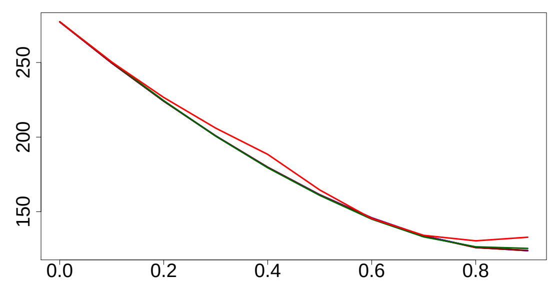

Compare results for different cut off value ε

- Ising model, 50×50 lattice
- Simulate first a realisation from the Ising model
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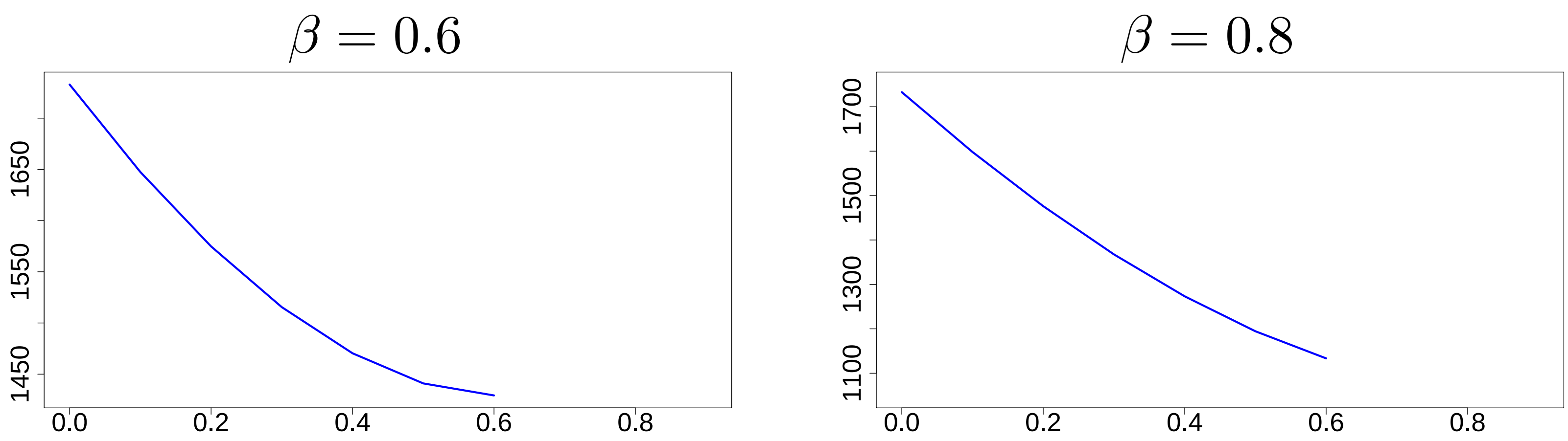
- Results for $\varepsilon = 10^{-5}$, 10^{-4}, 10^{-3}, 10^{-2} and 10^{-1}



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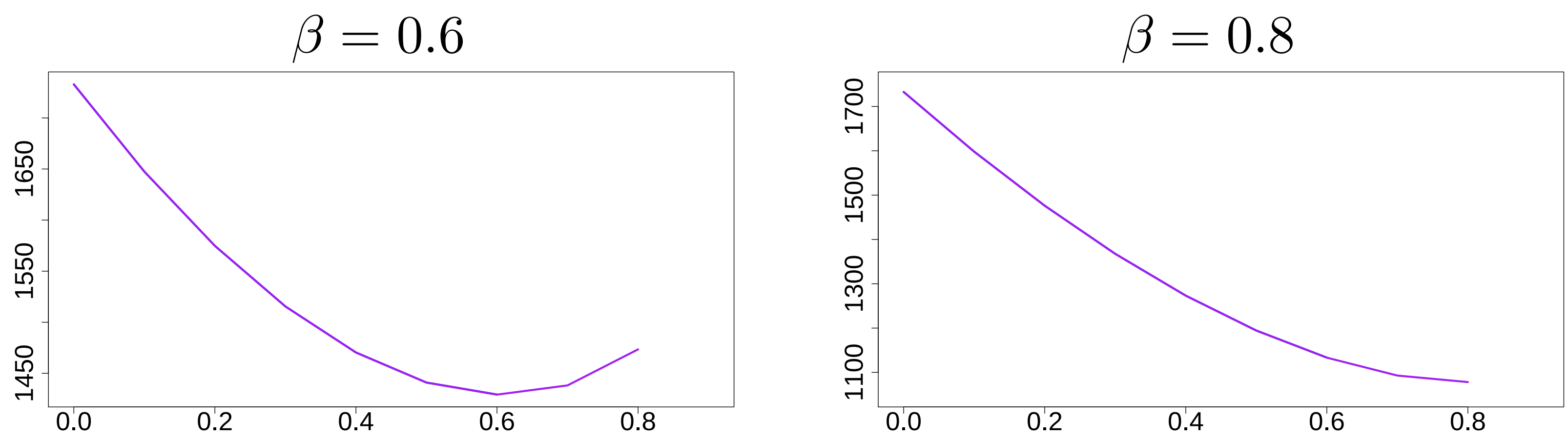

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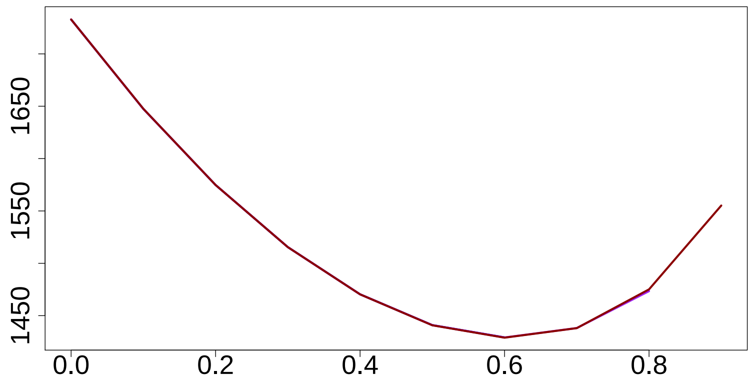

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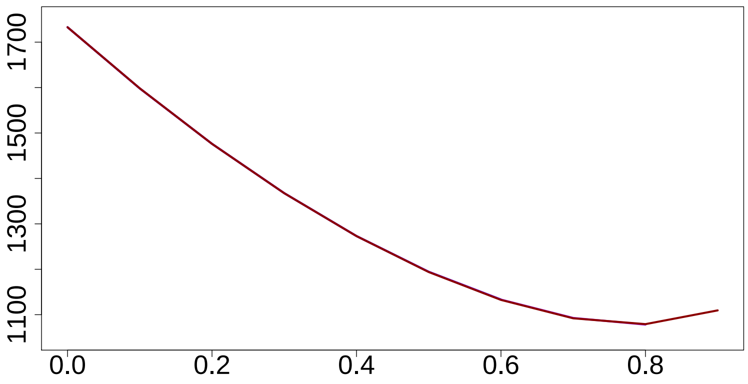

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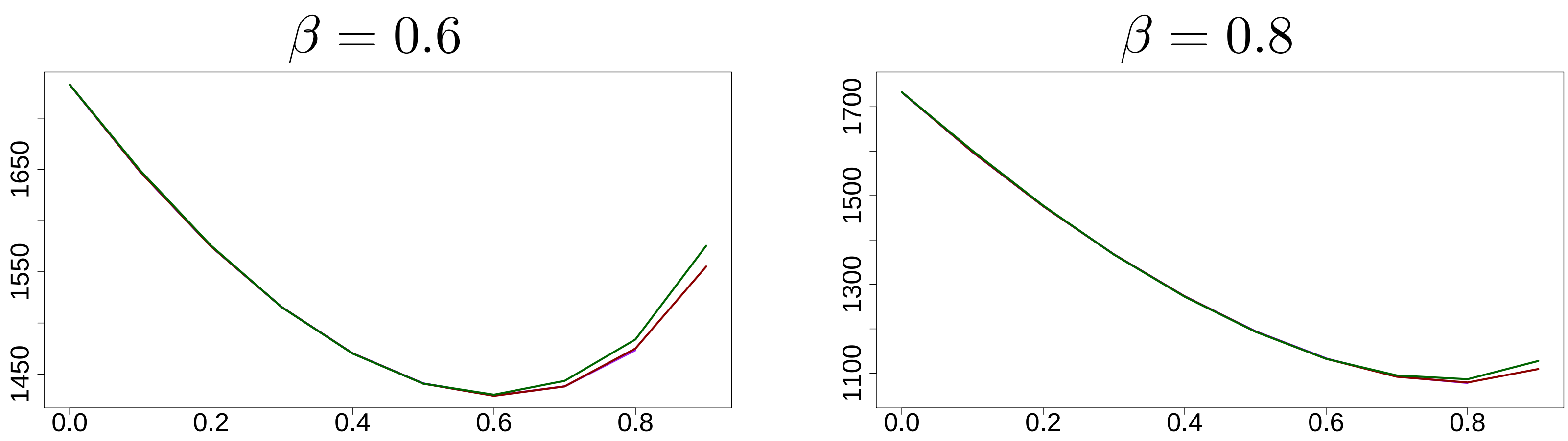

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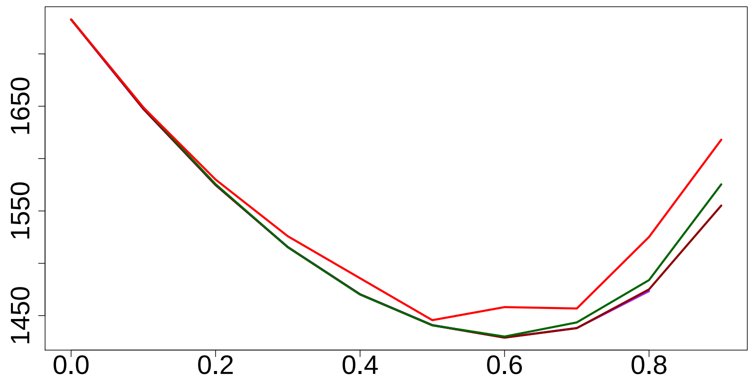

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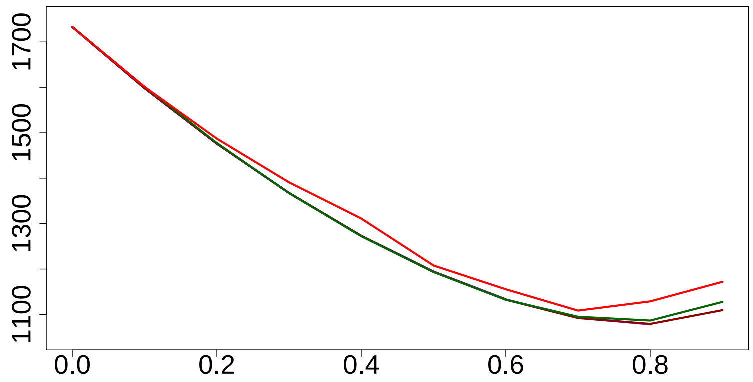

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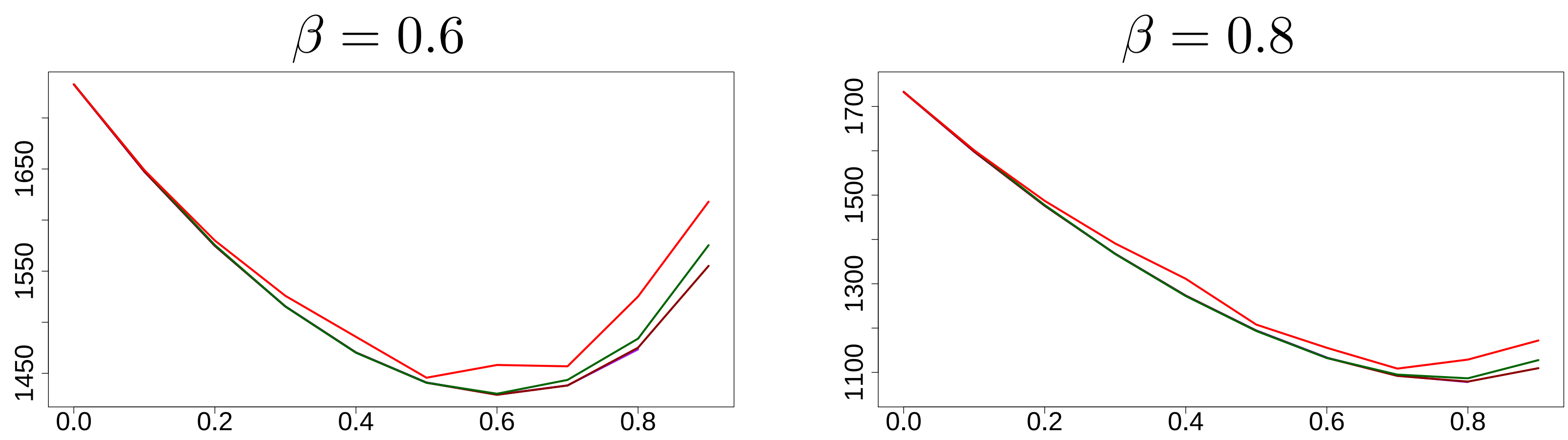


- Fraction of interactions computed for $\varepsilon = 10^{-3}$

β	0.1	0.3	0.5	0.7	0.9
fraction	$2.1 \cdot 10^{-13}$	$5.0 \cdot 10^{-12}$	$7.0 \cdot 10^{-12}$	$3.3 \cdot 10^{-11}$	$1.5 \cdot 10^{-10}$

Used as proposal in a Metropolis–Hastings algorithm

- Ising model, 50×50 lattice
- Initiate Metropolis–Hastings algorithm with exact sample
- Run for $\varepsilon = 10^{-1}$, 10^{-2}, 10^{-3}, 10^{-4} and 10^{-5}
- Monitor the Metropolis–Hastings acceptance rate

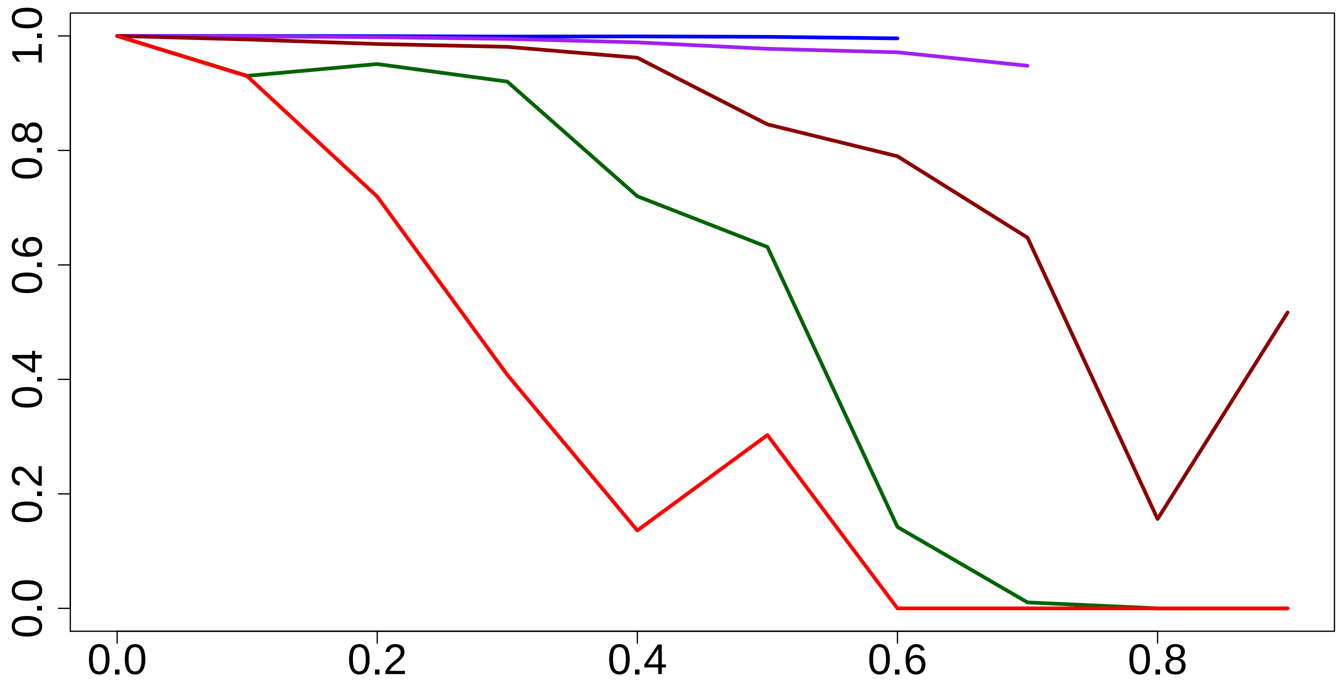
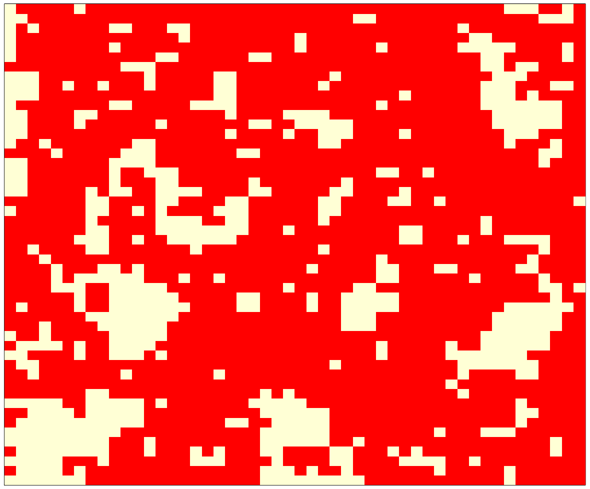


Image analysis example

- Ising prior, 50×50 lattice
- Conditionally independent Gaussian observations, $y_i|x_i \sim \mathrm{N}(x_i, \sigma^2)$
- Simulated data (true parameter values $\beta = 0.8$, $\sigma = 0.5$)
- Compute marginal likelihood function

$$l(\theta) = \pi(y|\theta) = \frac{\pi(x|\theta)\pi(y|x,\theta)}{\pi(x|y,\theta)}$$



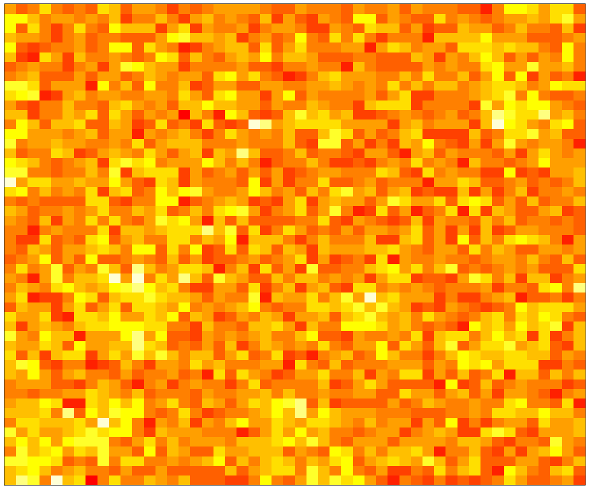
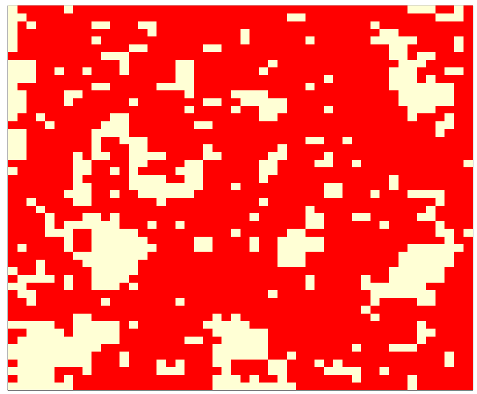
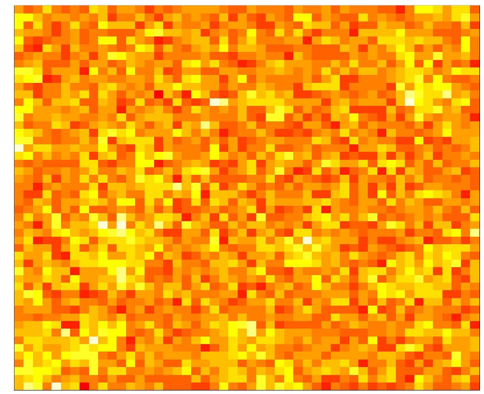
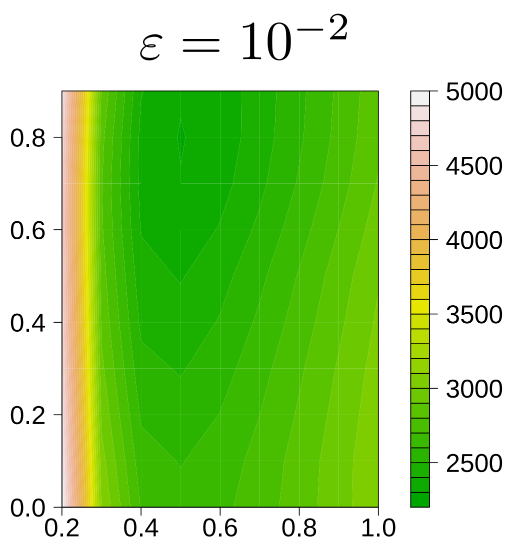
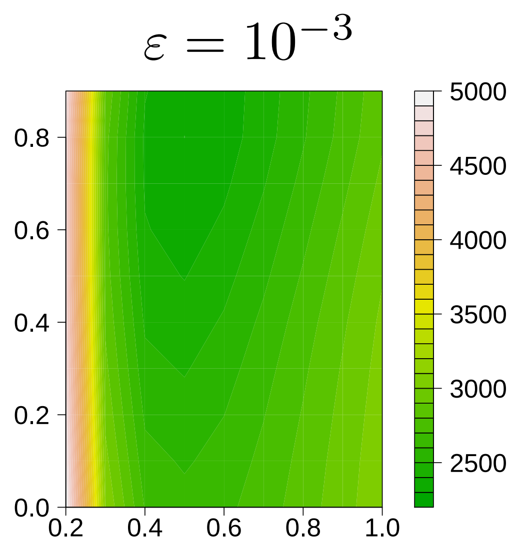


Image analysis example (cont.)









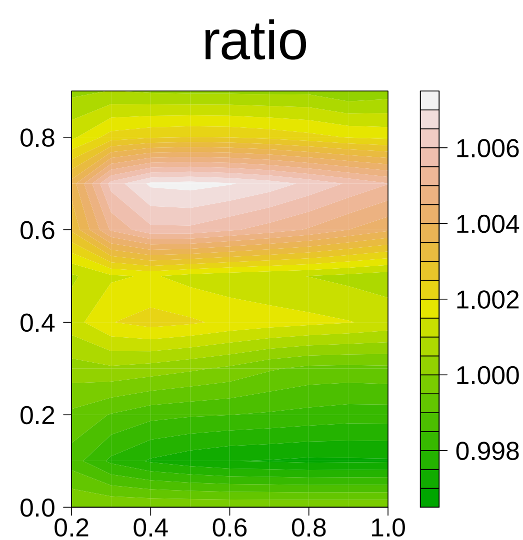
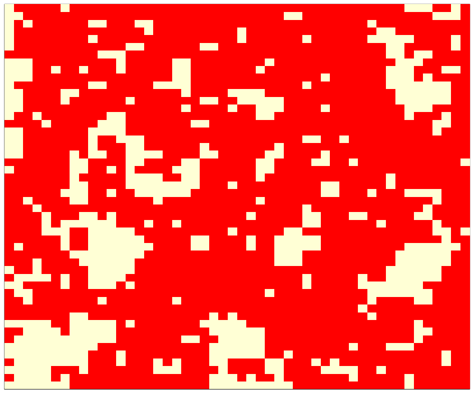
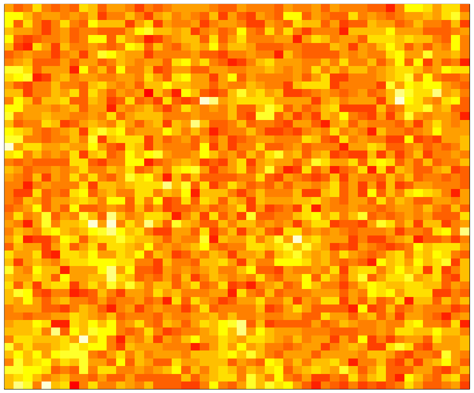
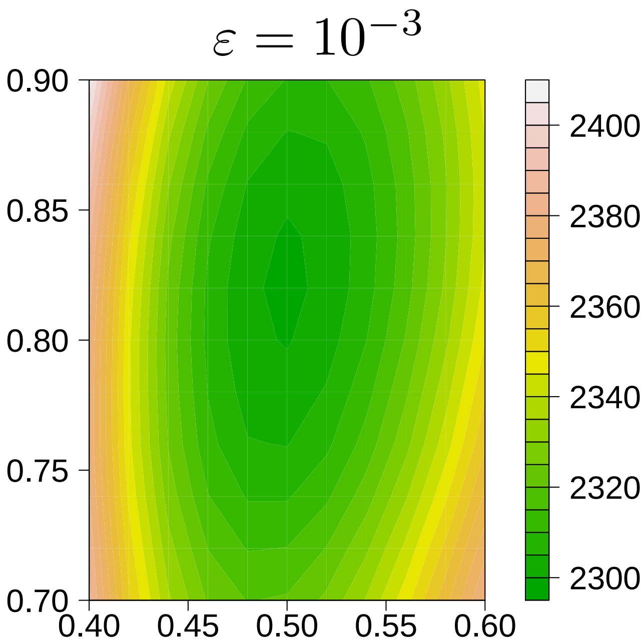


Image analysis example (cont.)

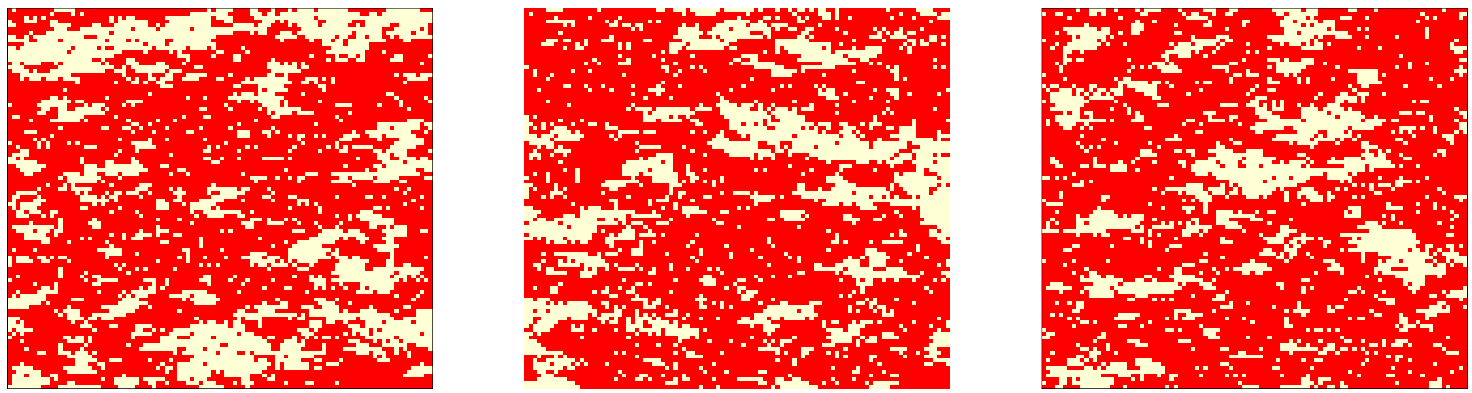




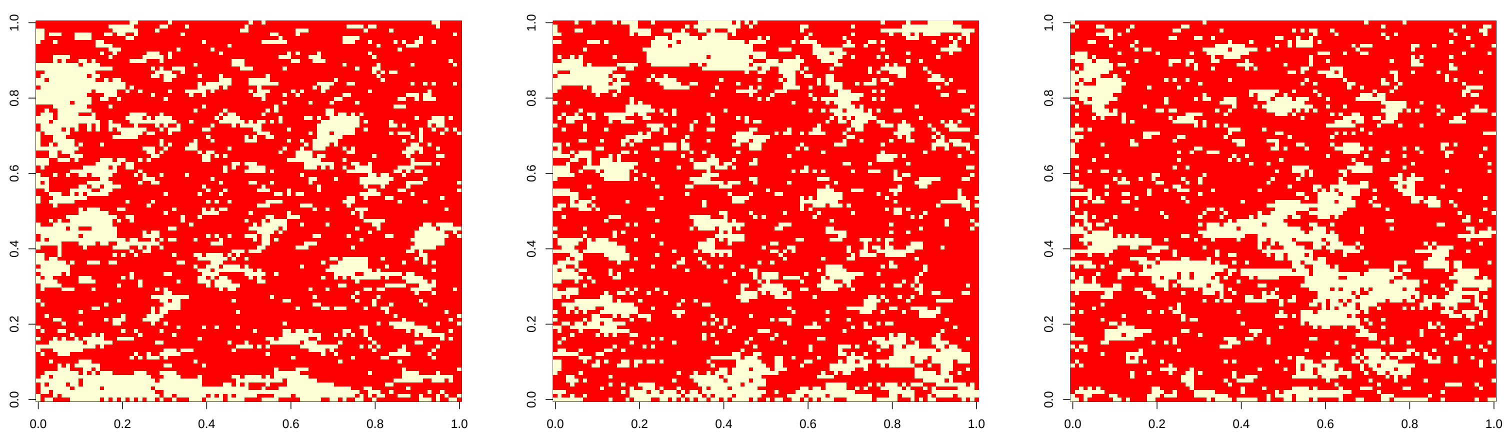


Example with 3×3 clique

- 3×3 clique model, pairwise interaction only, 100×100 lattice
- Realisations from specified model, by MCMC

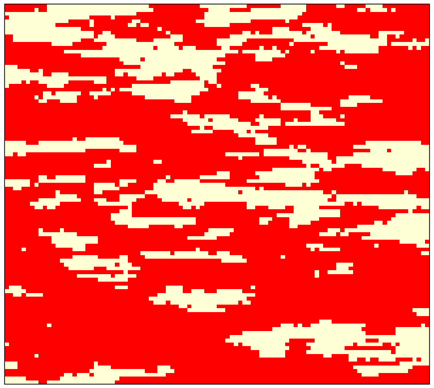
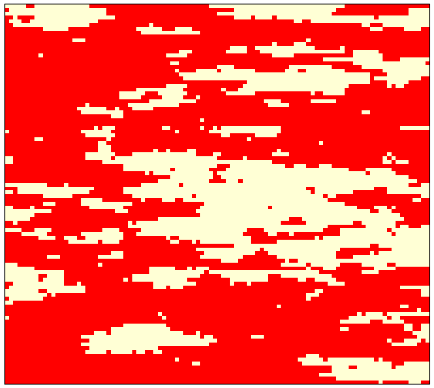
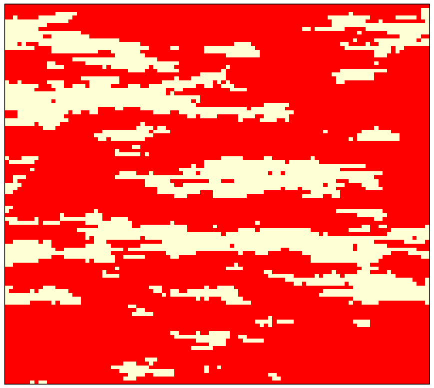


- Realisations from approximate model, $\varepsilon = 10^{-3}$



Problematic example

- 4×4 clique, strong higher order interactions
- Realisations from the model, by MCMC

- Too few interactions are approximated to zero — not able to run the approximation

A closer look at the approximate model

- Approximate model is

$$\widetilde{\pi}(x_{1:n}|\theta) = \widetilde{\pi}(x_n|\theta)\widetilde{\pi}(x_{n-1}|x_n, \theta)\widetilde{\pi}(x_{n-2}|x_{n-1:n}, \theta) \cdot \ldots \cdot \widetilde{\pi}(x_1|x_{2:n}, \theta)$$

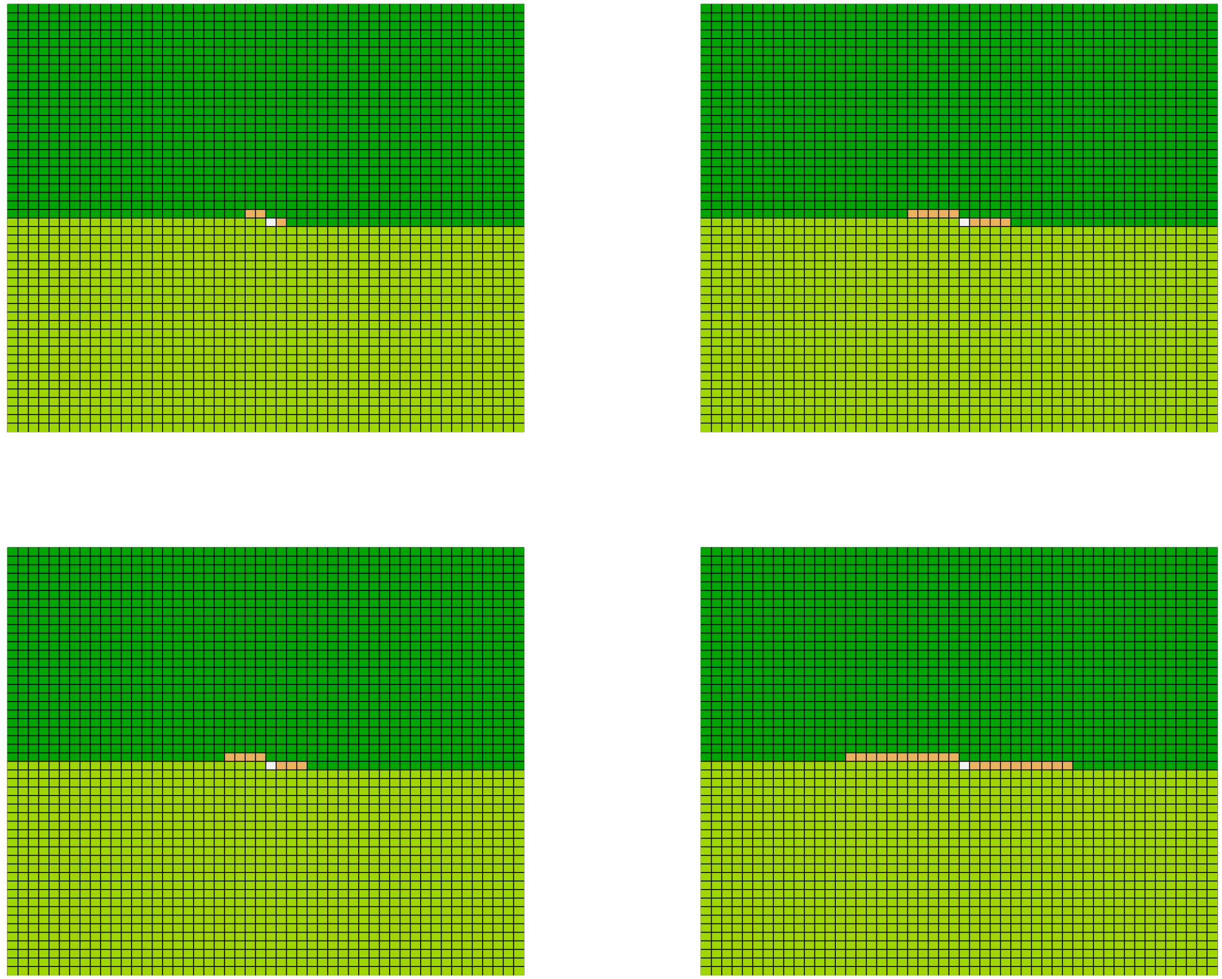
- Conditionally independence because:
  - original MRF
  - approximation

A closer look at the approximate model (cont.)

$\varepsilon = 10^{-2}$ | $\varepsilon = 10^{-4}$

$\beta = 0.4$

$\beta = 0.8$



Closing remarks

- For MRFs we have defined approximation to
  - the normalising constant — that (often) can be computed
  - the joint distribution — that (often) can be simulated directly
- The approximation is based on
  - representation of $b_k(x_{k:k+p}, \theta)$ by interaction parameters
  - most interaction parameters must be small
  - have assumed higher order interactions to be small whenever lower order interactions are small
- We have demonstrated the quality of the approximation in a number of examples
- The approximative model is a Markov mesh model (and POMM)
- Can sum out the variables in a different order