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Surveillance of spatial patterns

Change of interaction in the Ising model

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SURVEILLANCE OF SPATIAL PATTERNS

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ABSTRACT

Surveillance to detect changes of spatial patterns is of interest in many areas such as environmental control and regional analysis. Here the interaction parameter of the Ising model, is considered. A minimal sufficient statistic and its asymptotic distribution are used. It is demonstrated that earlier results on surveillance of a normally distributed random variable can be used for interesting cases. Properties such as expected delay and false alarm are examined for some examples.

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INTRODUCTION

Due to several environmental issues, such as radiation change detection, forestry disease surveillance, earthquake warning system, climate change detection and others, results about methods for judging whether a change in the behaviour of a spatial process has occurred or not, are strongly demanded. Two different approaches are

- **CHANGEPOINT ANALYSIS** The data consists of a realisation of the whole process and the surveillance task is to detect whether or not a change has occurred.
- **SURVEILLANCE** The data accumulates in time and it is decided "online" whether or not a change has occurred yet.

In this paper we will only be dealing with the latter of these two. For further reading see e.g. Basseville and Nikiforov [1], Frisén [4], Frisén and de Maré [5], Frisén and Wessman [6], Lai [13] or Wessman [31].

Quite recently Rogerson [24] investigated surveillance systems for monitoring the development of spatial patterns. Rogerson made an overview of surveillance approaches to the study of spatial clustering and concluded that they were rare. His suggestion was to use the cusum stopping rule of an index (Tango statistic) to detect a change in clustering. Rudemo and Tsybakov [26] analysed spatial change-point models for two-segment images with a linear boundary. Asymptotic distributions for piece-wise constant contour estimators for data of change-point type was examined by Rudemo and Stryhn [25] and spatial change-point models with application to image segmentation by Stryhn [29]. Tsybakov [30] considered changes of contours in image analysis and in point processes. The former area was also studied by Martin and Scott [15] and the latter by Le, Petkau and Rosychuk [14]. All these studies dealt with change-point problems in point processes.

In this paper we deal with a finite Markov random field denoted by X distributed according to the Ising model with zero exterior field. The reason for considering this model is that it is a simple non-trivial spatial interaction model and an investigation of this should therefore be a first step towards treating more sophisticated change point problems concerned with spatial data. We think of $X(1), \dots, X(t)$ as a development of X through the times $1, \dots, t$. Supposing there is a change in the interaction parameter of the distribution of X at a random time point and that the sequence of observations $X(1), X(2), \dots$ are conditionally independent given the time of change, we want to establish appropriate methods for detecting that change as soon and as accurately as possible after it has happened.

For this purpose, some statistic which reflects the amount of interaction, is of interest. One could use an estimator of the parameter, such as the maximum likelihood which has good properties as an estimator. We use another statistic sufficient for the interaction parameter. This means that no information reduction is made. We concentrate upon a minimal sufficient statistic which is approximately normally distributed for large lattice sizes. Since methods for surveillance of normal random variables are well studied problems (especially for the case when there is only a change in the expected value), many properties of the methods for surveillance of this statistic have been examined. Thus, the situations to which the methods of surveillance of univariate normal random variables apply, can be extended to include the problem of change of interaction in the Ising model with zero exterior field for large lattice sizes.

The paper is organized as follows: in Section 1 we will be treating spatial matters and in Sections 2 and 3, spatial surveillance.

1 SPATIAL MODEL

1.1 Markov Random Field

We briefly introduce the spatial model, Markov random field (MRF). A more thorough presentation of MRF's can be found in e.g. Kindermann and Snell [12] or Møller [16].

Let $A_n = \{1, 2, \dots, n^2\}$ be a finite set consisting of n^2 positions, called

	1	2	...	n
1	1	2	...	n
2	n+1	n+2	...	2n
...
n	n(n-1)+1	n(n-1)+2	...	n ²

Figure 1: *The $n \times n$ lattice A_n .*

sites, forming an $n \times n$ square lattice in \mathbb{Z}^2 (as shown in Figure 1). Each site possesses one of two possible states, 0 or 1. The configuration space

is a product space $E = \{0, 1\}^{n^2}$ with a σ -algebra, \mathcal{E} , of all possible subsets of E . Let $X = \{X_i\}_{i \in A_n}$ be a stochastic process on some probability space $(\Omega, \mathcal{F}, \mathbb{P})$ formed by the random variables $X_i : \Omega \rightarrow \{0, 1\}$ where $i \in A_n$. If $B \subset A_n$, we denote $\{X_i\}_{i \in B}$ by X_B . Since A_n is finite, so is E . X is assumed to have a distribution with density $p(x)$ (where x denote a realisation of X) with respect to the counting measure on E . For convenience, we assume the positivity condition which, according to Besag [2], is due to Hammersley and Clifford [10] and is defined as follows.

DEFINITION 1 *The stochastic process $X = \{X_i\}_{i \in A_n}$ is said to fulfill a POSITIVITY CONDITION if $\mathbb{P}[X_i = x_i] > 0$ for each $i \in A_n$ implies that $\mathbb{P}[X_1 = x_1, \dots, X_{n^2} = x_{n^2}] > 0$.*

DEFINITION 2 *A NEIGHBOURHOOD RELATION is a relation, denoted by \sim , such that $i \not\sim i$ and $i \sim j \Rightarrow j \sim i$ for each $i, j \in A_n$. The sites i and j are then called NEIGHBOURS.*

One may define different neighbourhood relations. We define that two sites are neighbours, $i \sim j$, if $\|i - j\| = 1$, where $\|\cdot\|$ denotes the Euclidean distance (see Figure 2). Then the sites i and j are called FIRST ORDER NEIGHBOURS.

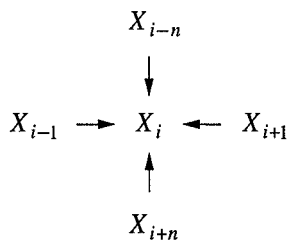


Figure 2: A site i has four neighbours, $i-n$, $i-1$, $i+1$, $i+n$. Therefore, a state X_i depends on its neighbouring states X_{i-n} , X_{i-1} , X_{i+1} and X_{i+n} .

DEFINITION 3 *The NEIGHBOURHOOD of i is the set $\partial i = \{j \in A_n : i \sim j\}$.*

DEFINITION 4 *A stochastic process $X = \{X_i\}_{i \in A_n}$ is called a MARKOV RANDOM FIELD if*

$$\mathbb{P}[X_i = x_i \mid X_{A_n \setminus \{i\}} = x_{A_n \setminus \{i\}}] = \mathbb{P}[X_i = x_i \mid X_{\partial i} = x_{\partial i}] \quad (1)$$

for each $i \in A_n$ and $x \in E$.

The conditional distributions in (1) are called LOCAL CHARACTERISTICS and (1) is called the MARKOV PROPERTY. It can be shown that a Markov random field is uniquely determined by its local characteristics (Møller [16]).

1.2 Ising Model

For this first study of spatial surveillance, we would like to consider a simple spatial model. Later, extensions of it may be made for more applicable models. The two-dimensional Ising model with zero exterior field (by Pickard called the most simple non-trivial case [22]) is a simple MRF model with the non-trivial characteristic of phase transition.

Let us first define some general concepts.

DEFINITION 5 *A non-empty set C of sites in A_n is called a CLIQUE if C consists of a single site or if $j \sim i$ for each distinct $i, j \in C$. The family of all cliques of A_n is denoted by \mathcal{C} .*

Thus, in an MRF with first order neighbours, all cliques are of size 1 or 2.

DEFINITION 6 *X is a GIBBS PROCESS if its distribution is of the form $p(x; \theta) = Z^{-1} \exp(-U(x; \theta))$, where $Z = \sum_{y \in E} \exp(-U(y; \theta))$ is a NORMALIZING CONSTANT (or partition function), $U(x; \theta) = \sum_{C \in \mathcal{C}} V_C(x; \theta)$ is the ENERGY FUNCTION and all functions $V_C(x; \theta) : E \times \Theta \rightarrow \mathbb{R}$ (called POTENTIALS) depend on x only through x_C . θ is a parameter vector in the distribution p with values in the parameter space Θ .*

Due to the fundamental *Hammersley-Clifford theorem*, inference in MRF's is much simplified.

THEOREM 1 (HAMMERSLEY-CLIFFORD) *X is a Markov random field iff X is a Gibbs process.*

The original proof can (according to Besag [2] who himself gives an alternative proof) be found in Hammersley and Clifford [10].

DEFINITION 7 *The ISING MODEL WITH ZERO EXTERIOR FIELD is a special case of the distribution of the Gibbs process $p(x; \phi)$ with potential functions*

$$V_C(x; \phi) = \begin{cases} \phi I(x_i = x_j) & \text{whenever } C = \{i, j\} \\ 0 & \text{whenever } C \text{ is a single site} \end{cases}$$

where C is a clique, ϕ is a real valued parameter and $I(L)$ is an indicator function, i.e. unity whenever L is true and zero otherwise.

Since the Ising model is so simple, we may write the distribution as

$$p(x; \phi) = \frac{1}{Z} \exp \left(-\phi \sum_{i \in A_n} \sum_{j \in \partial i: j < i} I(x_i = x_j) \right)$$

where $Z = Z(\phi) = \sum_{y \in E} \exp \left(-\phi \sum_{i \in A_n} \sum_{j \in \partial i: j < i} I(x_i = x_j) \right)$.

The value of the interaction parameter ϕ tells us whether we are likely to get an attractive or a repulsive pattern. When ϕ is negative the neighbours tend to have the same values and when ϕ is positive then the neighbouring sites tend to have different values. The ultimate attraction case corresponds to configurations with all states alike, either 0's or 1's. The ultimate repulsion case corresponds to "chessboard configurations". The condition $j < i$, in the summation index in the energy function, fixes the pair-potential sum so that we only count an interaction contribution once. This is equivalent to letting $U(x; \phi) = \frac{\phi}{2} \sum_{i \in A_n} \sum_{j \in \partial i} I(x_i = x_j)$.

This model is essentially the model in Besag [2] and Ising [12]. Most commonly the possible states are -1 and 1 and the energy is $U(x; \phi) = \phi \sum_{i \in A_n} \sum_{j \in \partial i: j < i} x_i x_j$. These settings are equivalent to ours. Besag, on the other hand, combines the state space $\{0, 1\}$ with an energy $U(x; \phi) = \phi \sum_{i \in A_n} \sum_{j \in \partial i: j < i} x_i x_j$ which therefore gives rise to a little different situation.

Let $\xi_i(x) = \sum_{j \in A_n \setminus i} \sum_{k \in A_n \setminus i: k < j} I(x_j = x_k)$. Then the LOCAL CONDITIONAL DISTRIBUTION, given the neighbourhood, is

$$\begin{aligned} p_{X_i | X_{\partial i}}(x_i | x_{\partial i}; \phi) &= \frac{\mathbb{P}[X = x]}{\mathbb{P}[X_{A_n \setminus i} = x_{A_n \setminus i}]} = \frac{\frac{1}{Z} \exp(-U(x; \phi))}{\frac{1}{Z} \sum_{x_i \in \{0, 1\}} \exp(-U(x; \phi))} \\ &= \frac{\exp \left(-\phi \xi_i(x) - \phi \sum_{j \in \partial i} I(x_i = x_j) \right)}{\exp \left(-\phi \xi_i(x) - \phi \sum_{j \in \partial i} I(x_j = 0) \right) + \exp \left(-\phi \xi_i(x) - \phi \sum_{j \in \partial i} I(x_j = 1) \right)} \\ &= \frac{\exp \left(-\phi \sum_{j \in \partial i} I(x_i = x_j) \right)}{\exp \left(-\phi \sum_{j \in \partial i} I(x_j = 0) \right) + \exp \left(-\phi \sum_{j \in \partial i} I(x_j = 1) \right)} = \frac{1}{Z_i} \exp \left(-\phi \sum_{j \in \partial i} I(x_i = x_j) \right) \end{aligned}$$

where $Z_i = e^{-\phi \sum_{j \in \partial i} I(x_j = 0)} + e^{-\phi \sum_{j \in \partial i} I(x_j = 1)}$ is the LOCAL NORMALIZING CONSTANT.

REMARK Let us consider the special cases with one neighbourhood consisting of only 0's denoted by $\{0, 0, 0, 0\}$ and another of only 1's $\{1, 1, 1, 1\}$. Then

$$\begin{aligned} p_{X_i | X_{\partial i}}(0 | \{0, 0, 0, 0\}; \phi) &\rightarrow \begin{cases} 1 & \text{as } \phi \rightarrow -\infty \\ 0 & \text{as } \phi \rightarrow \infty \end{cases} \\ p_{X_i | X_{\partial i}}(0 | \{1, 1, 1, 1\}; \phi) &\rightarrow \begin{cases} 0 & \text{as } \phi \rightarrow -\infty \\ 1 & \text{as } \phi \rightarrow \infty \end{cases} \end{aligned}$$

which might serve as an illustration to the *fact* that in the Ising model

$$\phi = -\infty \Rightarrow X_i = X_j \text{ a.s. for all } i, j \in A_n \quad (2)$$

and

$$\phi = \infty \Rightarrow X_i \neq X_j \text{ a.s. for all } i \in A_n, j \in \partial i. \quad (3)$$

A major feature of the Ising model concerns the random variable $\frac{1}{n^2} \sum_{i \in A_n} X_i$. The conditional distribution of X_i , given $X_{\partial i}$, is unique for all values of

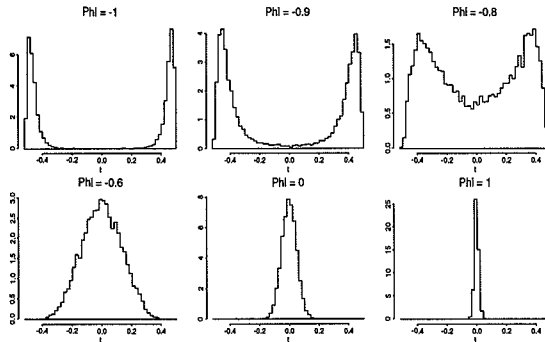


Figure 3: Empirical distribution of $\frac{1}{2} - \frac{1}{100} \sum_{i \in A_{10}} X_i$ (the centered average number of 1's in an Ising pattern X) for some values of ϕ based on 5000 simulations of X .

ϕ . However, for ϕ negative large enough, i.e. $\phi < \phi_- \approx -0.88$, the limit distribution of $\frac{1}{n^2} \sum_{i \in A_n} X_i$ as n tends to infinity is not unique (its empirical distribution for the 10×10 -lattice is shown in Figure 3), Kindermann and Snell [12]. This phenomenon is called PHASE TRANSITION and it is, according to Kindermann and Snell, characterized by the limit result proved by Georgii [8]: as n tends to infinity

$$\frac{1}{n^2} \sum_{i \in A_n} X_i \xrightarrow{\mathcal{D}} \begin{cases} \frac{1}{2} \left(1 + (1 - \sinh^{-4} \phi)^{\frac{1}{8}} \right) & \text{w.p. } \frac{1}{2} \\ \frac{1}{2} \left(1 - (1 - \sinh^{-4} \phi)^{\frac{1}{8}} \right) & \text{w.p. } \frac{1}{2} \end{cases} \text{ if } \phi < \phi_-$$

$$\frac{1}{2} \text{ if } \phi > \phi_-$$

as plotted in Figure 4. (One can also prove a similar result for $\phi > 0$, Kindermann and Snell [12].)

The result (2) can be proved in the case of a square lattice MRF simply by taking the distribution of the random variable $\lim_{n \rightarrow \infty} \frac{1}{n^2} \sum_{i \in A_n} X_i$ to the limit as $\phi \rightarrow -\infty$. For the second claim (3), consider an attractive Ising configuration. A pattern with the same amount of repulsion may be achieved

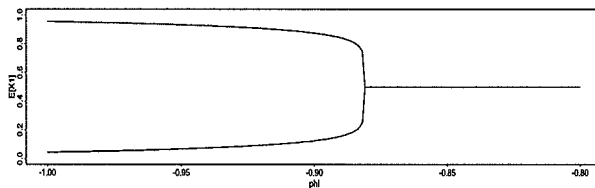


Figure 4: $\lim_{n \rightarrow \infty} \frac{1}{n^2} \sum_{i \in A_n} X_i$ plotted against ϕ .

by switching all states at odd sites of an attractive configuration: trade x_i for $1-x_i$. Then the previous result implies the result in (3). More formally, decomposing A_n into A'_n and A''_n (see Figure 5), one observes that the energy

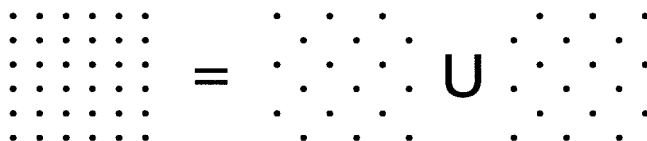


Figure 5: Partition of A_n into A'_n and A''_n .

function for $X \stackrel{\mathcal{D}}{=} p(x; \phi)$ is just

$$\begin{aligned} U(x; \phi) &= \phi \sum_{i \in A_n} \sum_{j \in \partial i: j < i} \mathbb{I}(x_i = x_j) \\ &= \frac{\phi}{2} \sum_{i \in A'_n} \sum_{j \in \partial i} \left(1 - \mathbb{I}(x_i = 1 - x_j)\right) + \frac{\phi}{2} \sum_{i \in A''_n} \sum_{j \in \partial i} \left(1 - \mathbb{I}(1 - x_i = x_j)\right) \\ &= 2n^2\phi - U(x_{A'_n} \cup (J_n - x)_{A''_n}; -\phi) \end{aligned}$$

where J_n means the $n \times n$ configuration of all 1's. Therefore $p(x; \phi) = p(x_{A'_n} \cup (J_n - x)_{A''_n}; -\phi)$ since the first term, $2n^2\phi$, in the last expression cancels out against the same contribution from the normalizing constant. Since $X_i = 1 - X_j$ a.s. in our case with 0-1-states is the same as $X_i \neq X_j$ a.s., (2) implies (3).

1.3 ML Estimation of the Interaction Parameter

For surveillance of ϕ , some statistic which reflects the amount of interaction in a realisation x of X , is of interest. One idea is that if there is a change in ϕ , this could be recognized as a shift of an estimator of ϕ . Therefore we focus on the maximum likelihood (ML) estimator in this section.

The maximum likelihood estimator of ϕ is the value that maximizes the likelihood function

$$L(\phi; x) = \frac{\exp\left(-\phi \sum_{i \in A_n} \sum_{j \in \partial i: j < i} I(x_i = x_j)\right)}{\sum_{y \in E} \exp\left(-\phi \sum_{i \in A_n} \sum_{j \in \partial i: j < i} I(y_i = y_j)\right)}$$

and the log likelihood function

$$l(\phi; x) = -\phi \sum_{i \in A_n} \sum_{j \in \partial i: j < i} I(x_i = x_j) - \log\left(\sum_{y \in E} \exp\left(-\phi \sum_{i \in A_n} \sum_{j \in \partial i: j < i} I(y_i = y_j)\right)\right).$$

In short this is to say that we want to solve the equation

$$\sum_{i \in A_n} \sum_{j \in \partial i: j < i} I(x_i = x_j) = \mathbb{E}_\phi \left[\sum_{i \in A_n} \sum_{j \in \partial i: j < i} I(X_i = X_j) \right] \quad (4)$$

with respect to ϕ . The maximum likelihood estimator has been proved to be consistent and asymptotically normal (Besag [3]). However the expected value on the right hand side of the equation (4) cannot be calculated analytically (except for very small lattice sizes, and even then the explicit forms are horrifying) since we would have to go through all 2^{n^2} possible realisations of X . Some successful efforts have been made to find an approximate maximum likelihood estimator (see e.g. Geyer and Thompson [9]) but this does not change the fact that such an estimator of ϕ is only available as an *implicit* solution of an equation.

1.4 Sufficient Statistic

If we could find a statistic sufficient for ϕ we would not need any estimator for surveillance. Therefore, let us recall the global distribution of X

$$p(x; \phi) = \frac{1}{Z} \exp\left(-\phi \sum_{i \in A_n} \sum_{j \in \partial i: j < i} I(x_i = x_j)\right)$$

which is a member of the exponential family.

DEFINITION 8

$$S_n = \frac{1}{n^2} \sum_{i \in A_n} \sum_{j \in \partial i: j < i} I(X_i = X_j)$$

Of course S_n is a.s. on the closed interval $[0, 2]$ for any values of n and ϕ . Low values of S_n indicate repulsion and large values attraction.

OBSERVATION 1 S_n is minimal sufficient for ϕ .

Since the Ising model is an exponential family member, this is immediate.

1.4.1 Limit Moments

For surveillance of ϕ based upon S_n , we need to know the distribution of S_n . For $\phi=0$ we have that $P[X_i=0] = P[X_i=1] = 1/2$ for each $i = 1, 2, \dots, n^2$ implying that

$$n^2 S_n = \sum_{i \in A_n} \sum_{j \in \partial i: j < i} I(X_i = X_j) \stackrel{D}{=} \text{Bin}(1/2, 2n^2). \quad (5)$$

The distribution of S_n when $\phi \neq 0$ is not as simple to derive. It has been shown that S_n is asymptotically normal (Pickard [21]). The moments of S_n are possible to calculate directly only for very small lattice sizes $n \times n$ since, in order to calculate the normalizing constant, one has to go through all 2^{n^2} possible configurations in E . Let us, for approximate values of the first and second moments, turn to the limit moments of S_n for a while and then return to the finite case which is what we are interested in.

To get a first idea of $\lim_{n \rightarrow \infty} E_\phi[S_n]$ one may derive from (2), (3) and (5) that

$$\begin{aligned} \phi = -\infty &\Rightarrow X_i \stackrel{a.s.}{=} X_j \text{ for all } i, j \in A_n \Rightarrow \lim_{n \rightarrow \infty} E_{-\infty}[S_n] = 2 \\ \phi = 0 &\Rightarrow X_i, X_j \text{ independent} \Rightarrow \lim_{n \rightarrow \infty} E_0[S_n] = 1 \\ \phi = \infty &\Rightarrow X_i \stackrel{a.s.}{\neq} X_j \text{ for all } i \in A_n, j \in \partial i \Rightarrow \lim_{n \rightarrow \infty} E_\infty[S_n] = 0. \end{aligned}$$

From these three values one may roughly guess how $\lim_{n \rightarrow \infty} E_\phi[S_n]$ looks but, as we shall see, there is one important feature of this limit which maybe is not immediately discernible.

Let us recall the derivation of the expected value and variance of S_n (Pickard [21]). Let $Z_n(\phi)$ be the normalizing constant in the $n \times n$ lattice Ising model with zero exterior field.

$$\text{OBSERVATION 2} \quad n^2 E_\phi[S_n] = -\frac{d}{d\phi} \log Z_n(\phi) \quad n^4 \text{Var}_\phi[S_n] = \frac{d^2}{d\phi^2} \log Z_n(\phi).$$

Differentiating $\log Z_n(\phi)$ with respect to ϕ , we see that

$$\begin{aligned} \frac{d}{d\phi} \left(-\log Z_n(\phi) \right) &= -\frac{1}{Z_n(\phi)} \cdot \frac{d}{d\phi} \sum_{x \in E} \exp(-\phi n^2 S_n) \\ &= \frac{1}{Z_n(\phi)} \sum_{x \in E} n^2 S_n \exp(-\phi n^2 S_n) \\ &= n^2 E_\phi[S_n] \end{aligned}$$

$$\begin{aligned}
\frac{d^2}{d\phi^2} \left(\log Z_n(\phi) \right) &= \frac{d}{d\phi} \left(-\frac{1}{Z_n(\phi)} \sum_{x \in E} n^2 S_n \exp(-\phi n^2 S_n) \right) \\
&= \frac{\sum n^4 S_n^2 \exp(-\phi n^2 S_n)}{Z_n(\phi)} + \frac{\sum n^2 S_n \exp(-\phi n^2 S_n)}{Z_n(\phi)^2} \cdot \frac{d}{d\phi} Z_n(\phi) \\
&= n^4 \text{Var}_\phi[S_n].
\end{aligned}$$

The limit $\zeta(\phi) = \lim_{n \rightarrow \infty} \log Z_n(\phi)/n^2$ may be calculated explicitly in terms of ϕ (Onsager [18]) as

$$\begin{aligned}
\zeta(\phi) &= \lim_{n \rightarrow \infty} \frac{\log Z_n(\phi)}{n^2} = \\
&\underbrace{\log \left(\frac{2}{(1+\psi)^2} \right)}_{\zeta_1(\phi)} + \frac{1}{8\pi^2} \int_0^{2\pi} \int_0^{2\pi} \underbrace{\log \left((1+\psi^2)^2 + 2\psi(1-\psi^2)(\cos u + \cos v) \right)}_{\zeta_2(\phi, u, v)} du dv
\end{aligned}$$

where $\psi = \tanh \frac{\phi}{2}$. Observe the removable singularities at $\cos u = \cos v = 1$, $\psi = \sqrt{2} \pm 1$ i.e. $\phi = \pm \log(\sqrt{2} - 1)$, the critical values, ϕ_- and ϕ_+ , of the parameter at which phase transition occurs! ζ and the first derivative of ζ with respect to ϕ , ζ' , are continuous on the lot of \mathbb{R} while the second derivative of ζ with respect to ϕ , ζ'' , is continuous on $\mathbb{R} \setminus \{\phi_-, \phi_+\}$. Let us restrict to the case where $\phi \in (\phi_-, \phi_+)$. Then $\lim_{n \rightarrow \infty} \frac{\log Z_n(\phi)}{n^2} = \zeta(\phi)$ and $\frac{d}{d\phi} \left(\frac{\log Z_n(\phi)}{n^2} \right)$, $\frac{d^2}{d\phi^2} \left(\frac{\log Z_n(\phi)}{n^2} \right)$ are continuous and tend uniformly to $\zeta'(\phi)$ and $\zeta''(\phi)$, respectively. We have

$$\lim_{n \rightarrow \infty} \mathbf{E}_\phi[S_n] = -\frac{d}{d\phi} \left(\lim_{n \rightarrow \infty} \frac{\log Z_n(\phi)}{n^2} \right) = -\frac{d\zeta_1}{d\phi} - \frac{1}{8\pi^2} \int_0^{2\pi} \int_0^{2\pi} \frac{d\zeta_2}{d\phi} du dv$$

(Plotted in Figure 6.)

$$\lim_{n \rightarrow \infty} n^2 \text{Var}_\phi[S_n] = \frac{d^2}{d\phi^2} \left(\lim_{n \rightarrow \infty} \frac{\log Z_n(\phi)}{n^2} \right) = \frac{d^2\zeta_1}{d\phi^2} + \frac{1}{8\pi^2} \int_0^{2\pi} \int_0^{2\pi} \frac{d^2\zeta_2}{d\phi^2} du dv$$

(Plotted in Figure 7.)

Due to Proposition 1, which follows below, it suffices to look at negative values of ϕ for statements about S_n regarding the expectation and variance.

DEFINITION 9 *A function $f : D \rightarrow \mathbb{R}$ is called EVEN (ODD) if $f(x) = f(-x)$ ($f(x) = -f(-x)$) for each x in D .*

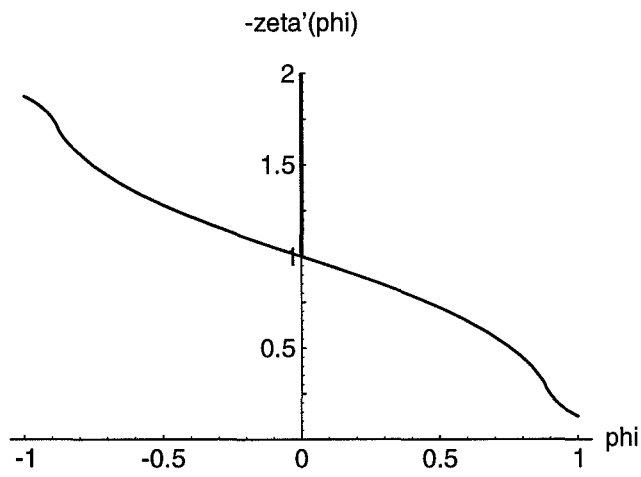


Figure 6: A plot of $-\zeta'(\phi) = \lim_{n \rightarrow \infty} E_{\phi}[S_n]$.

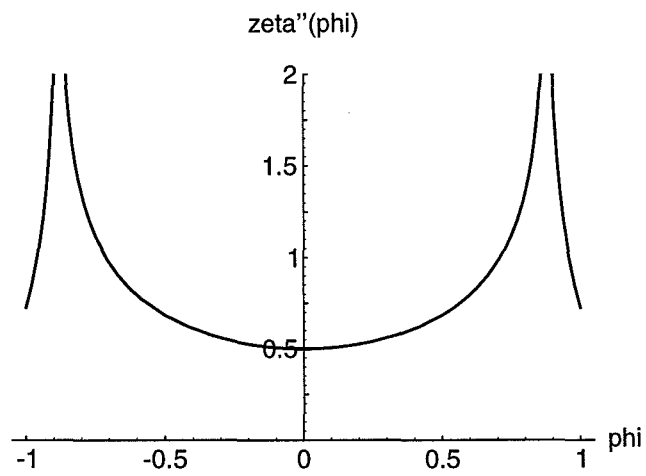


Figure 7: A plot of $\zeta''(\phi) = \lim_{n \rightarrow \infty} n^2 \text{Var}_{\phi}[S_n]$.

PROPOSITION 1 $E_\phi[S_n]-1$ is an odd function of ϕ . $\text{Var}_\phi[S_n]$ is even.

PROOF In subsection 1.2 we deduced that

$$U(x; \phi) = 2n^2\phi - U(x_{A'_n} \cup (J_n - x)_{A''_n}; -\phi).$$

Since $U(x; \phi) = n^2\phi S_n(x)$ we have that

$$\begin{aligned} E_\phi[S_n] &= \sum_{x \in E} S_n(y(x)) \frac{\exp(-U(y(x); \phi))}{Z_n(\phi)} \\ &\quad (\text{where } y(x) = x_{A'_n} \cup (J_n - x)_{A''_n}) \\ &= \sum_{x \in E} (2 - S_n(x)) \frac{\exp(-2n^2\phi + U(x; -\phi))}{\sum_{z \in E} \exp(-2n^2\phi + U(z; -\phi))} \\ &= 2 - E_{-\phi}[S_n] \end{aligned}$$

so $E_\phi[S_n]-1 = -(E_{-\phi}[S_n]-1)$ for each $\phi \in \mathbb{R}$.

$\text{Var}_\phi[S_n]$ is even since it is the derivative of $-n^{-2}E_\phi[S_n]$ with respect to ϕ .

□

Much of the research of MRF's has been concentrated upon events concerned with the phase transition region and questions about what happens as ϕ approaches the critical values from the positive and the negative sides. As it happens, the situations that most call for methods of surveillance are when there is a *small* change of the parameter in focus, meaning that the local behaviour of $\lim_{n \rightarrow \infty} E_\phi[S_n]$ and $\lim_{n \rightarrow \infty} \text{Var}_\phi[S_n]$ is of interest. As well, for many situations, at first, there might be no interaction but we want to know if/when the sequence of Ising patterns suddenly are starting to show attraction or repulsion.

To summarize, we want to know some local properties of $\lim_{n \rightarrow \infty} E_\phi[S_n]$ and $\lim_{n \rightarrow \infty} \text{Var}_\phi[S_n]$ about the origin. For this purpose, a result that will prove to be useful for surveillance later on, is the following.

PROPOSITION 2 $\lim_{n \rightarrow \infty} E_\phi[S_n] = 1 - \frac{\phi}{2} + \mathcal{O}(\tilde{\phi}^3)$ $\lim_{n \rightarrow \infty} n^2 \text{Var}_\phi[S_n] = \frac{1}{2} + \mathcal{O}(\tilde{\phi}^2)$
where $\tilde{\phi} \in (\phi, 0)$.

PROOF Let

$$\zeta(\phi) = \lim_{n \rightarrow \infty} \frac{\log Z_n(\phi)}{n^2} = \zeta_1(\phi) + \frac{1}{8\pi^2} \int_0^{2\pi} \int_0^{2\pi} \zeta_2(\phi, u, v) du dv$$

as given previously in this subsection. From direct calculation we have that $\zeta(0) = \log 2$ and from (5), that $\zeta'(0) = -1$. Differentiating ζ_1 twice, we get

$$\zeta_1''(\phi) = -\frac{2\psi''(1+\psi) - 2(\psi')^2}{(1+\psi)^2} \quad \text{where } \psi = \tanh \frac{\phi}{2}.$$

Since

$$\psi' = \frac{1}{2 \cosh^2 \frac{\phi}{2}} \quad \text{and} \quad \psi'' = -\frac{\tanh \frac{\phi}{2}}{2 \cosh^2 \frac{\phi}{2}} = -\psi \psi'$$

we have $\psi''' = (-\psi \psi')' = -(\psi')^2 - \psi^2 \psi'$ and $\psi(0) = 0$, $\psi'(0) = \frac{1}{2}$, $\psi''(0) = 0$ so $\psi'''(0) = -\frac{1}{4}$ and $\zeta_1''(0) = \frac{1}{2}$. Differentiating ζ_1'' reveals that

$$\zeta_1'''(0) = -\frac{\psi'}{1+\psi} \left(\psi^2 + \psi \psi' - 2\psi' + \frac{4\psi'}{1+\psi} \left(\psi + \frac{\psi'}{1+\psi} \right) \right) \Big|_{\phi=0} = 0.$$

Tedious differentiation of ζ_2 w.r.t. ϕ shows that

$$\frac{d^2}{d\phi^2} \zeta_2(\phi, u, v) \Big|_{\phi=0} = 1 - (\cos u + \cos v)^2$$

and

$$\frac{d^3}{d\phi^3} \zeta_2(\phi, u, v) \Big|_{\phi=0} = (\cos u + \cos v) \left(2(\cos u + \cos v)^2 - 5 \right)$$

implying $\frac{d^2}{d\phi^2} \int_0^{2\pi} \int_0^{2\pi} \zeta_2(\phi, u, v) du dv \Big|_{\phi=0} = \frac{d^3}{d\phi^3} \int_0^{2\pi} \int_0^{2\pi} \zeta_2(\phi, u, v) du dv \Big|_{\phi=0} = 0$ and thus we have

$$\zeta''(0) = \frac{1}{2} \quad \text{and} \quad \zeta'''(0) = 0.$$

Finally, by Taylor expansion about the origin,

$$\zeta(\phi) = \log 2 - \phi + \frac{\phi^2}{4} + \mathcal{O}(\tilde{\phi}^4)$$

so that

$$-\zeta'(\phi) = 1 - \frac{\phi}{2} + \mathcal{O}(\tilde{\phi}^3) \quad \text{and} \quad \zeta''(\phi) = \frac{1}{2} + \mathcal{O}(\tilde{\phi}^2).$$

where $\tilde{\phi} \in (\phi, 0)$.

□

1.4.2 Asymptotic Normality

To conduct surveillance of S_n , we need to know its distribution.

THEOREM 2 (CENTRAL LIMIT THEOREM FOR THE ISING MODEL)

If $\phi \in (\phi_-, \phi_+)$, then

$$\frac{S_n - E_\phi[S_n]}{\sqrt{\text{Var}_\phi[S_n]}} \xrightarrow{\mathcal{D}} N(0, 1) \quad \text{as } n \rightarrow \infty$$

A detailed proof for this is given by Pickard [21].

REMARK According to Theorem 2 we have approximately, for large lattice sizes $n \times n$, that

$$S_n \stackrel{\mathcal{D}}{=} N(-\zeta'(\phi), \zeta''(\phi)/n^2) \quad (6)$$

for all $\phi \in (\phi_-, \phi_+)$.

Let us look at the empirical distribution of S_n for some different lattice sizes n and some values of the interaction parameter ϕ . One measurement of discrepancy between empirical distribution and approximate distribution values is the KOLMOGOROV STATISTIC. We denote it by $K = \sup_s |\tilde{F}_N(s) - F(s)|$ where $\tilde{F}_N(s)$ is the empirical distribution of S_n from a simulated sample of S_n of size N and $F(s)$ the normal distribution with mean $-\zeta'(\phi)$ and variance $\zeta''(\phi)/n^2$.

EXAMPLE 1 The convergence towards normal distribution is very rapid. From 10 000 simulations of a 4×4 lattice Ising model with $\phi = -0.35$, we see the empirical distribution of S_4 in Figure 8 where $K = 0.11$. As we shall see later, a change from $\phi = 0$ to $\phi = -0.35$ in a 4×4 lattice corresponds to a change in mean from 0 to 1.

Another example which corresponds to a change in mean from 0 to 1 is a 10×10 lattice when ϕ changes from 0 to -0.14 and here $K = 0.06$, an improvement due to both larger lattice size and ϕ closer to the origin. The empirical distribution of S_{10} with $\phi = -0.14$ is shown in Figure 9.

Convergence towards the normal distribution is slower for ϕ closer to the points of phase transition (e.g. the left point ϕ_-), and in spite of a larger lattice size (resulting in a smoother empirical distribution) there is some systematic deviance from the normal distribution. In Figure 10 is an example with $\phi = -0.8$ and $n = 20$ where $K = 0.05$. The normal approximation works better the larger the lattice size (of course) and the closer to the origin the interaction parameter.

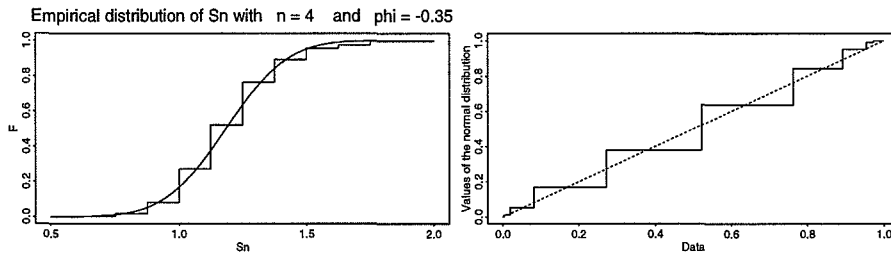


Figure 8: *Left picture: empirical distribution of S_4 when $\phi = -0.35$. Right picture: Values of the empirical distribution plotted against the values of a normal distribution with mean $-\zeta'(-0.35) \approx 1.18$ and variance $0.0625 \zeta''(-0.35) \approx 0.036$.*

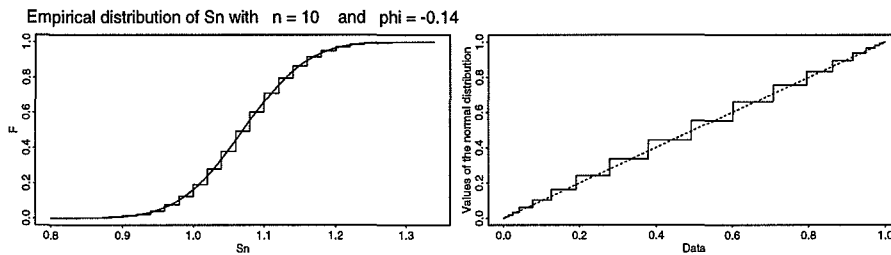


Figure 9: *Left picture: empirical distribution of S_{10} when $\phi = -0.14$. Right picture: the values of the empirical distribution plotted against the values of a normal distribution with mean $-\zeta'(-0.14) \approx 1.07$ and variance $0.01 \zeta''(-0.14) \approx 0.005$.*

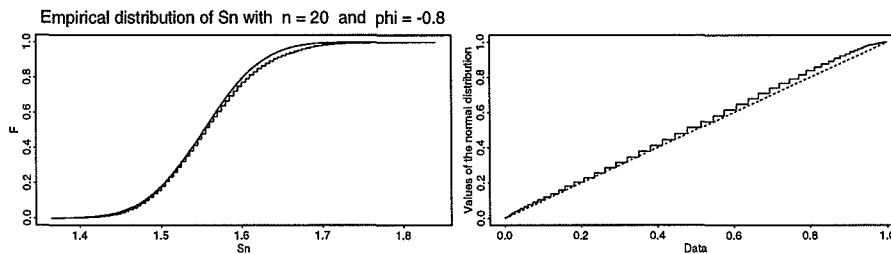


Figure 10: *Left picture: empirical distribution of S_{20} when $\phi = -0.8$. Right picture: the values of the empirical distribution plotted against the values of a normal distribution with mean $-\zeta'(-0.8) \approx 1.55$ and variance $0.0025 \zeta''(-0.8) \approx 0.003$. There is some systematic deviance of the empirical distribution from the normal.*

2 SURVEILLANCE

Henceforth we denote an Ising configuration occurring at time t by $X(t) = \{X_i(t) : i \in A_n\}$ and we assume that

$$\mathbb{P}[X(t) = x(t) \mid X(t-1) = x(t-1), \dots, X(1) = x(1), \tau = u] = \mathbb{P}[X(t) = x(t) \mid \tau = u]$$

which implies that the $S_n(t)$'s are conditionally independent given τ . We make observations of $\{X_i(t)\}_{t \in \mathbb{N}, i \in A_n}$, a sequence of Ising model patterns $\{X(1), \dots, X(t)\}$, where

$$X(t) \stackrel{\mathcal{D}}{=} \begin{cases} p(x(t); \phi_0) & \text{if } t < \tau \\ p(x(t); \phi_1) & \text{if } t \geq \tau \end{cases}$$

where the distribution $p(\cdot; \phi)$ is as given in Section 1.2 and $\phi_0, \phi_1 \in (\phi_-, \phi_+)$. We consider the problem of detecting a change of ϕ from ϕ_0 to ϕ_1 .

The suggested method of surveillance will be based on the minimal sufficient statistic

$$\tilde{S}_n(t) = \frac{S_n(t) - \mathbf{E}_{\phi_0}[S_n(t)]}{\sqrt{\text{Var}_{\phi_0}[S_n(t)]}}$$

which for large n , due to the asymptotic normality of $S_n(t)$, is approximately normal

$$\tilde{S}_n(t) \stackrel{\mathcal{D}}{=} \begin{cases} \text{N}(0, 1) & \text{if } t < \tau \\ \text{N}(\mu, \sigma) & \text{if } t \geq \tau \end{cases}$$

where $\mu = n(-\zeta'(\phi_1) + \zeta'(\phi_0)) / \sqrt{\zeta''(\phi_0)}$ and $\sigma = \sqrt{\zeta''(\phi_1) / \zeta''(\phi_0)}$.

When ϕ changes from ϕ_0 to ϕ_1 , there is a simultaneous change in both $\mathbf{E}_\phi[\tilde{S}_n(t)]$ and $\text{Var}_\phi[\tilde{S}_n(t)]$. However, if both ϕ_0 and ϕ_1 are in a small interval about the origin, the variance of $\tilde{S}_n(t)$ is close to a constant with respect to ϕ , i.e. $\tilde{S}_n(t)$ is approximately distributed $\text{N}(0, 1)$ for $t < \tau$, $\text{N}(\mu, 1)$ for $t \geq \tau$. Let us concentrate upon this situation.

2.1 Accuracy of Approximations

Since the situation of change from independence to slight interaction is an important special case, we focus some extra upon this. To get an idea of how large n needs to be and how close to 0 ϕ_0 and ϕ_1 should be, let us look at some examples. The accuracy of the approximation with the normal distribution was illustrated in Section 1.4.2.

Let us recall Proposition 2,

$$\lim_{n \rightarrow \infty} \mathbb{E}_\phi[S_n] = 1 - \phi/2 + \mathcal{O}(\tilde{\phi}^3) \quad \text{and} \quad \lim_{n \rightarrow \infty} n^2 \text{Var}_\phi[S_n] = 1/2 + \mathcal{O}(\tilde{\phi}^2),$$

where $\tilde{\phi} \in (\phi, 0)$. Due to this, $\sigma^2 = (1/2 + \mathcal{O}(\tilde{\phi}_1^2))/(1/2 + \mathcal{O}(\tilde{\phi}_0^2))$, which is not a function of n (since we have normed $S_n(t)$ with its standard deviation). This variance is approximately 1 for ϕ_0, ϕ_1 close to 0 (see Table 1).

ϕ_1	-0.5	-0.45	-0.4	-0.35	-0.3	-0.25	-0.2	-0.15	-0.1	-0.05	0
σ^2	1.370	1.288	1.221	1.165	1.118	1.081	1.051	1.028	1.013	1.003	1.000

Table 1: Values of $\sigma^2 = \text{Var}_{\phi_1}[\tilde{S}_n(t)]$ for different ϕ_1 when $\phi_0 = 0$.

The linear transformation $\tilde{S}_n(t) = n(S_n(t) + \zeta'(\phi_0)) / \sqrt{\zeta''(\phi_0)}$ also makes the expected value of $\tilde{S}_n(t)$ after change

$$\mu = \mathbb{E}_{\phi_1}[\tilde{S}_n(t)] \approx n(-\zeta'(\phi_1) + \zeta'(\phi_0)) / \sqrt{\zeta''(\phi_0)}. \quad (7)$$

For a picture of this relation between n, ϕ_1 and μ , when $\phi_0 = 0$ we have the following table of values of ϕ_1 such that (7) holds.

In Table 2, looking down the 4th column, it says that if we are interested in a change corresponding to that from $N(0, 1)$ to $N(1, 1)$, it is only for lattice sizes larger than 14×14 that ϕ_1 is less than 0.1 away from the origin which in turn, by Table 1, guarantees the variance after change to be less than 1.013 which might be approximated by 1 for some level of accuracy.

We summarize this section with the following conclusion.

COROLLARY 1 *For ϕ_0, ϕ_1 close to the origin and large n , the normal distribution approximates the distribution of $\tilde{S}_n(t)$ well. The surveillance problem of shift from ϕ_0 to ϕ_1 can be reduced to a problem of monitoring a shift in the mean of a normal distribution.*

It is important that the condition " ϕ_0, ϕ_1 close to the origin " is fulfilled in order for the variance approximation to be sensible. This is illustrated by the next example.

EXAMPLE 3 Recalling the Kolmogorov statistic $K = \sup_s |\tilde{F}_N(s) - F(s)|$, let us look at the empirical distributions of \tilde{S}_n when $\phi = \phi_1$. Suppose that $\phi_0 = 0$ and $\phi_1 = -0.8$, not close to the origin but rather close to ϕ_- . Then variance

μ	0.1	0.25	0.5	1	2
n					
5	-0.028	-0.071	-0.142	-0.274	-0.513
6	-0.024	-0.059	-0.117	-0.230	-0.434
7	-0.020	-0.050	-0.101	-0.199	-0.380
8	-0.018	-0.044	-0.088	-0.175	-0.337
9	-0.016	-0.039	-0.078	-0.156	-0.304
10	-0.014	-0.035	-0.071	-0.142	-0.274
11	-0.013	-0.032	-0.064	-0.128	-0.250
12	-0.012	-0.029	-0.059	-0.117	-0.230
13	-0.011	-0.027	-0.054	-0.108	-0.212
14	-0.010	-0.025	-0.050	-0.101	-0.197
15	-0.009	-0.024	-0.047	-0.094	-0.188
16	-0.009	-0.022	-0.044	-0.088	-0.176
17	-0.008	-0.021	-0.041	-0.083	-0.166
18	-0.008	-0.020	-0.039	-0.078	-0.157
19	-0.007	-0.019	-0.037	-0.074	-0.148
20	-0.007	-0.018	-0.035	-0.071	-0.142
50	-0.003	-0.007	-0.014	-0.028	-0.056
100	-0.001	-0.004	-0.007	-0.014	-0.028

Table 2: Values of ϕ_1 such that $E_{\phi_1}[\tilde{S}_n(t)] = \mu$ for different μ and n when $\phi_0 = 0$.

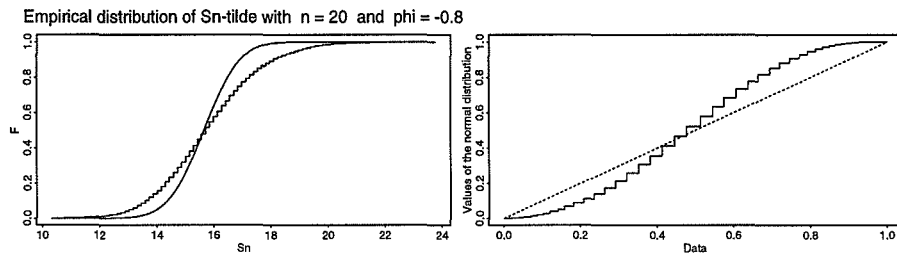


Figure 11: Left picture: empirical distribution of \tilde{S}_{20} when $\phi_1 = -0.8$. Right picture: the values of the empirical distribution plotted against the values of a normal distribution with mean $20 \cdot 2^{1/2}(-\zeta'(-0.8) - 1) \approx 15.6$ and variance 1 (a poor approximation of the real variance 2.7).

of \tilde{S}_{20} is $2\zeta''(-0.8) \approx 2.7$ quite far from 1. This is a case of simultaneous change in both μ and σ . If ϕ_1 is close to ϕ_- or ϕ_+ and a model with unit variance before and after change, is used, this gives poor accuracy for the method ($K=0.16$, in Example 1 we had $K=0.05$) as can be seen in Figure 11. This inaccuracy will remain no matter how large n is since the variance of \tilde{S}_n does not depend on n . However, this situation is not so important from a surveillance point of view since large n and a radical change of ϕ (from 0 to -0.8), which corresponds to a shift in mean of \tilde{S}_n from 0 to 15.6, would be immediately obvious to the eye of an observer and not *need* a method of surveillance.

2.2 Evaluation of the Procedure

There are several general surveillance methods suggested in the literature. The simplest is the Shewhart stopping rule, suggested by Shewhart [27],

$$T = \inf\{t \geq 1 : \tilde{S}_n(t) > c\}$$

where c is a constant.

Just looking at Table 1 and Table 2 may give the impression that, for instance, situations with $\phi_0=0$, $\phi_1=-0.14$ and $n=5, 10, 20$ are equivalent from a surveillance point of view. To see clearly that this is not the case, one could look at a measurement of how well a certain stopping rule behaves.

DEFINITION 10 *The expected stopping time given that no change occurs, $E[T | \tau = \infty]$, is called ARL^0 (AVERAGE RUNLENGTH). The expected time from change to stop given that the change has occurred by the stopping time, $E[T - \tau | T \geq \tau]$, is called EXPECTED DELAY.*

The expected delay has to do with delay of true alarm and ARL^0 has to do with probability of false alarm. Of course we want both these to be as small as possible but as they are somewhat contradictory, one has to settle with a little of both.

Let us look at the expected delay for a fixed level of ARL^0 . Denoting the cumulative distribution function before change $P_{\phi_0}[\tilde{S}_n(t) \leq s]$ by $F_0(s)$ and after change $P_{\phi_1}[\tilde{S}_n(t) \leq s]$ by $F_1(s)$, we recall that, for the Shewhart method, the average runlength is

$$ARL^0 = E[T | \tau = \infty] = \frac{1}{1 - F_0(c)}$$

and the expected delay

$$E[T - \tau | T \geq \tau] = \frac{F_1(c)}{1 - F_1(c)}$$

and thus the relation between average runlength and expected delay

$$\text{OBSERVATION 3 } E[T-\tau | T \geq \tau] = F_1(F_0^{-1}(\frac{ARL^0-1}{ARL^0})) / \left(1 - F_1(F_0^{-1}(\frac{ARL^0-1}{ARL^0}))\right).$$

Suppose that we fix the average runlength $ARL^0 = 100$. Then the values of expected delay of detection of a change from $\phi_0 = 0$ to $\phi_1 = -0.14$ when $n=5, 10, 20$ are the following.

$$\begin{aligned} n=5 &\Rightarrow \text{change of } \tilde{S}_n(t) \text{ from } N(0, 1) \text{ to } N(\frac{1}{2}, 1) \Rightarrow E[T-\tau | T \geq \tau] = 28.5 \\ n=10 &\Rightarrow \text{change of } \tilde{S}_n(t) \text{ from } N(0, 1) \text{ to } N(1, 1) \Rightarrow E[T-\tau | T \geq \tau] = 9.8 \\ n=20 &\Rightarrow \text{change of } \tilde{S}_n(t) \text{ from } N(0, 1) \text{ to } N(2, 1) \Rightarrow E[T-\tau | T \geq \tau] = 1.7 \end{aligned}$$

EXAMPLE 3 Suppose $\phi_0 = 0$, $\phi_1 = -0.14$ and $n = 10$. Figure 12 shows one realisation of the alarm function (in the Shewhart case the alarm function

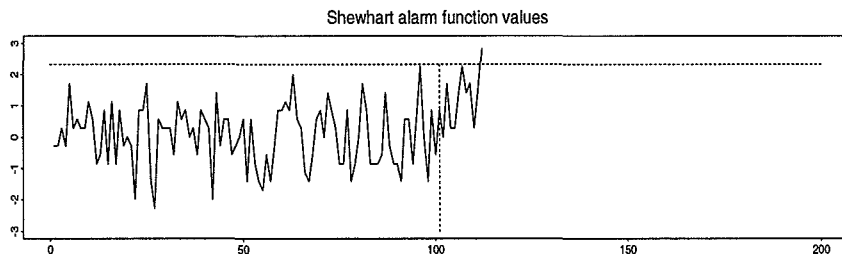


Figure 12: Values of the Shewhart alarm function for a simulated sequence of Ising configurations. The dashed horizontal line is the critical boundary c and the dashed vertical line at $t=101$ is the time of change. The surveillance stopped (i.e. the alarm function crossed c) at $t=109$ in this particular case.

is simply $\tilde{S}_n(t)$). It is based on one simulation $\{x(t)\}_{t=1}^{200}$ of Ising configurations $X(t) \stackrel{D}{=} p(x(t); 0)$, $t = 1, 2, \dots, 100$ and $X(t) \stackrel{D}{=} p(x(t); -0.14)$, $t = 101, 102, \dots, 200$ (i.e. with $\tau = 101$). The critical level is c chosen such that $ARL^0 = 100$.

3 DISCUSSION

This study shows that for many cases, surveillance of the interaction parameter for a sequence of finite square lattice Ising patterns with zero exterior field can be performed using known methods of surveillance.

When the values of the interaction parameter, before and after change, are close to the origin (i.e. the local states in the Ising patterns appear almost

independently), the surveillance problem can be reduced to a special case of a well studied univariate surveillance problem. Closer to the points of phase transition, the problem of a change in interaction concerns with a simultaneous change in both expectation and variance of the statistic \hat{S}_n .

In this paper, only the simplest surveillance method (the Shewhart method) is considered. However, other surveillance methods, such as cusum methods, Shiryaev-Roberts method, likelihood ratio methods, exponentially weighted moving average methods, can, of course, be applied here as well.

The spatial surveillance model is the Ising model for the spatial structure and conditional independence of Ising configurations at different timepoints given the time of change. The applicability of this model may be questioned. One should bear in mind, though, that this study is meant as a first step towards solving more relevant problems.

Sometimes, methods for treating a simultaneous change in both intensity and interaction are necessary. The reason for choosing the Ising model was that it is a simple model which nevertheless possesses a non-trivial property. An extension to a square lattice auto-normal model could be appropriate for a lot of situations and would be even simpler since it would lack the phase transition singularities. There is also the possibility of a non-zero exterior field. In this paper we have considered only change in the interaction parameter in a zero exterior field model.

There are many possibilities to use the results on how the spatial surveillance problem can be transformed. For example, if the statistic follows an auto-regressive process, then methods for surveillance of an auto-regressive process can be used (Pettersson [20]).

APPENDIX: SIMULATION

To simulate an Ising model we have chosen a technique of the type called EXACT SIMULATION (introduced by Propp and Wilson [23]) for the illus-

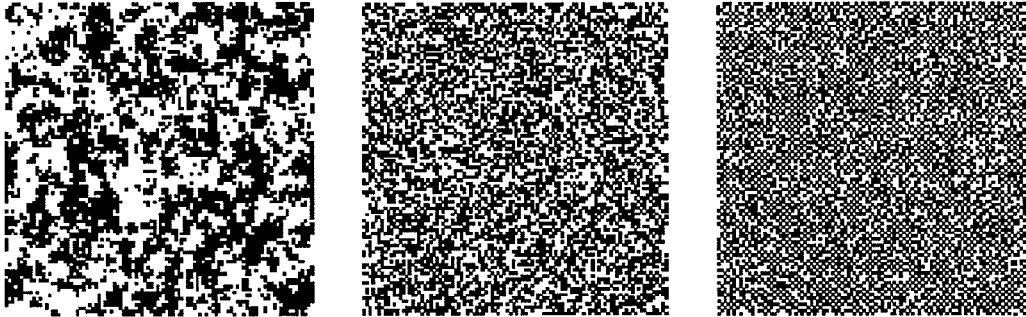


Figure 13: *Three 100×100 torus square lattice Markov random field realisations simulated exactly according to an Ising model, the first with interaction parameter $\phi = -0.7$, the second with $\phi = 0$ and the third with $\phi = 0.7$.*

tration of lattice realisations (see Figure 13). However, for large number of replicates this technique (in our implementation) is too time consuming for the computer. For the illustrations of the empirical distributions of the statistic, GIBBS SAMPLER was used. This is a well documented method for approximating samples from a Gibbs distribution.

Gibbs Sampler

The Gibbs sampler was invented by Suomela [28] but usually the credit goes to Geman and Geman [7]. It is a stepwise procedure where one, at each timestep $t = 1, 2, 3, \dots$, cruises along the sites $i \in A_n$ so that each site is almost surely visited infinitely often. This cruise could be made in a number of ways e.g. $i = 1, 2, \dots, n^2$. At each visit the state possessed by that site, is updated according to the map $g : E \times A_n \times [0, 1] \rightarrow E$ as

$$g(x(t), i, u_i(t)) = \begin{cases} x_{A_n \setminus i}(t) \cup \{1\} & \text{if } p_{X_i | X_{\partial i}}(1 | x_{\partial i}(t)) > u_i(t) \\ x_{A_n \setminus i}(t) \cup \{0\} & \text{otherwise} \end{cases}$$

where $\{u_i(t) : i = 1, \dots, n^2, t = 0, 1, 2, \dots\}$ is a sequence of independent observations of the uniform distribution on $[0, 1]$. For some fixed $t = t_0$, the states are $\{x_1(t_0), \dots, x_{n^2}(t_0)\}$. As all sites are visited and updated again the clock snaps one tick to $t = t_0 + 1$ and the states are $\{x_1(t_0 + 1), \dots, x_{n^2}(t_0 + 1)\}$, and

so on. Starting with arbitrary states $\{x_1(0), \dots, x_{n^2}(0)\}$ and updating according to this rule, the sequence $\{x(0), x(1), \dots\}$ of configurations achieved at each "full round", forms a Markov chain with the pleasing property that

$$P[X(t) = x \mid X(0) = x_0] \rightarrow p(x) \text{ as } t \rightarrow \infty \text{ for each } x, x_0 \in E$$

where p denotes the steady-state distribution of the Markov chain. So we may approximately simulate an Ising configuration according to the desired global distribution.

Exact Simulation

Let $\{u_i(t) : i = 1, \dots, n^2, t = -M, \dots, 0\}$ be a sequence of independent observations of a uniform random variable on $[0, 1]$. The main idea is the following: impose the partial ordering relation denoted by \preceq meaning that $x \preceq y$ if $x_i \leq y_i$ for each $i \in A_n$. Then generate two monotone Markov chains $\{x(t)\}_{t=-M}^0$ and $\{y(t)\}_{t=-M}^0$ according to the "Coupling-from-the-past-protocol" starting with $x(-M) = \hat{0}$ being the minimal state and $y(-M) = \hat{1}$ the maximal state and terminating with $x(0) = y(0)$ which is the simulated Ising configuration. The time $-M$ is unknown stochastic and it is determined during the evaluation of the algorithm. The algorithm is the pseudocode

```

T ← 1
repeat
  upper ←  $\hat{1}$ 
  lower ←  $\hat{0}$ 
  for t = -T to 0
    for i = 1 to  $n^2$ 
      upper ← g(upper, i,  $u_i(t)$ )
      lower ← g(lower, i,  $u_i(t)$ )
  T ← 2T
until upper = lower
return upper

```

where the map g may be chosen as the previous sampling algorithm Gibbs sampler or other Metropolis-Hastings algorithms (see Møller [17]) or some other that results in a Markov chain and which preserves the partial ordering.

However, the distribution p , that we want to simulate samples from, must satisfy a monotonicity condition (Propp and Wilson [23]) in order for the method to be valid. When ϕ is negative (attractive case), p is monotone but otherwise not. On the other hand, when ϕ is positive (repulsive case), p satisfies an anti-monotonicity condition and with a slight modification of the

updating map g , realisations can be simulated in this case as well (Häggström and Nelander [11]). In short this is to say, provided that we have chosen the Gibbs sampler as the map g in the case of positive ϕ , then the modification is just to update each site of say the chain referred to in the pseudocode as *upper*, not according to its neighbours but rather according to the corresponding neighbourhood of the partner chain *lower*. The same goes for updating each site of the *lower* chain according to the corresponding neighbourhood in the *upper* chain. Häggström and Nelander showed that this change makes the resulting Ising pattern distributed exactly according to the stationary distribution in the anti-monotone case. Thus we are able to simulate Ising configurations regardless of the value of ϕ .

As well it should be mentioned that we have avoided all edge problems by using the convention of a TORUS ALIGNMENT. This is to say: each edge site has as a neighbour the nearest site at the opposite edge and each corner site has as two neighbours the corner sites of the two nearby corners.

Program Code

We chose Fortran 77 using the NAG library for our simulation programs. Our implementation for exact simulation of the Ising model with zero exterior field now follows.

```

subroutine exact(rows,cols,
&    phi,lo,seed,loops)
external g05caf
external g05cbf
integer rows,cols,M,dlo1,
&    dhi1,seed,loops
&    lo(rows,cols),hi(rows,cols),
&    zeros(rows,cols),
&    ones(rows,cols),
double precision phi,
&    g05caf,prob.lo,prob.hi,
&    rands(rows,cols,loops)
logical coalesced
call g05cbf(seed)
do i=1,rows
  do j=1,cols
    zeros(i,j)=0
    ones(i,j)=1
    do m=1,loops
      rands(i,j,m)=
&        g05caf(rands(i,j,m))
      C
    end do
  end do
end do
do i=1,rows
  do j=1,cols
    zeros(i,j)=0
    ones(i,j)=1
  end do
end do
M=1
coalesced=.FALSE.
10 if(coalesced) goto 20
lo=zeros
hi=ones
call g05cbf(seed)
do k=1,M
  do i=1,rows
    do j=1,cols
      C
      TORUS ALIGNMENT
      if(i.gt.1) then
        i1=i-1
      else
        i1=rows
      endif
      if(j.lt.cols) then
        j2=j+1
      else
        j2=1
      endif
      if(i.lt.rows) then
        i3=i+1
      else
        i3=1
      endif
      C
      if(j.gt.1) then
        j4=j-1
      else
        j4=cols
      endif
      END TORUS ALIGNMENT
      COUNT NEIGHBOUR ZEROS AND ONES
      if(phi.le.0.d0) then
        dlo1=lo(i1,j)+lo(i,j2)+
&          lo(i3,j)+lo(i,j4)
        dhi1=hi(i1,j)+hi(i,j2)+
&          hi(i3,j)+hi(i,j4)
      else
        dlo1=hi(i1,j)+hi(i,j2)+
&          hi(i3,j)+hi(i,j4)
        dhi1=lo(i1,j)+lo(i,j2)+
&          lo(i3,j)+lo(i,j4)
      endif
      END COUNT NEIGHBOUR ZEROS AND ONES
      GIBBS SAMPLER
      prob.lo=1.d0/(1.d0+exp(
&        2.d0*phi*(dlo1-2.d0)))
      prob.hi=1.d0/(1.d0+exp(
&        2.d0*phi*(dhi1-2.d0)))
      if(prob.lo.gt.rands(i,j,
&        loops-k+1)) then
        lo(i,j)=1
      else
        lo(i,j)=0
      endif
      if(prob.hi.gt.rands(i,j,
&        loops-k+1)) then
        hi(i,j)=1
      else
        hi(i,j)=0
      endif
      END GIBBS SAMPLER
    end do
  end do
end do
SET COALESCED
coalesced=.TRUE.
do i=1,rows
  do j=1,cols
    coalesced=coalesced.and.
&      (lo(i,j).eq.hi(i,j))
  end do
end do
END SET COALESCED
M=2*M
goto 10
return
end

```


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