Potential estimation in the Ising model through Poisson approximations

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Abstract
A 2-dimensional Ising model on a square lattice torus is considered. Each vertex is an atom whose spin is either positive or negative. We are interested in the occurrences in the lattice of any given local configuration. Such configuration describes a finite set of positive vertices. We focus in particular on local configurations whose set of positive vertices is connected (with respect to 4-connectivity). These 4-connected components are known in the combinatorics literature as square lattice animals or polyominoes. As the size $n$ of the lattice tends to infinity, a Poisson approximation is given for the distribution of the number of occurrences in the lattice of any given local configuration, provided the surface potential $a = a(n)$ tends to $-\infty$ and the pair potential $b$ remains fixed. Applying this Poisson approximation to square lattice animals, an algorithm to estimate the potentials $a$ and $b$ is proposed, based both on the size and on the perimeter of square lattice animals.

Key words: Potential estimation, Ising model, Poisson approximations, square lattice animals.

AMS Subject Classification: 68U20, 60F05.
1 Introduction

Suppose \{I_\lambda\}_{\lambda \in \Lambda} is a finite family of indicator random variables, with the properties that the probabilities \( P(I_\lambda = 1) \) are small and that there is not too much dependence between the \( I_\lambda \)'s. Then, it is reasonable to expect the distribution of \( \sum_{\lambda \in \Lambda} I_\lambda \) to be approximately Poisson. In the theory of random graphs, such results are frequent: see e.g. Bollobás (1985) or Spencer (2001). The \( I_\lambda \) can, for instance, indicate the places in the random graph where a given subgraph appears. Some analogous results hold for random colorings of a lattice graph in dimension 2, corresponding to the context of random images: see Couplier et al. (2005). In the case where vertices are dependent random variables, namely the spins of an Ising model, some Poisson approximations have been established in Couplier (2005) and recalled here in part (i) of Theorem 3.1. Our goal is to illustrate this result and to study its statistical consequences.

Let us consider the vertex set \( V_n = \{0, \ldots, n-1\}^2 \). The integer \( n \) will be called the size of the lattice. It is embedded in \( \mathbb{Z}^2 \) and naturally endowed with a graph structure; the case of the 4-connectivity is considered. For \( i, j \geq 0 \), the neighbors of \((i, j)\) are:

\[
(i + 1, j), (i - 1, j), (i, j + 1), (i, j - 1)
\]

The fact that vertices \( x \) and \( y \) are neighbor will be denoted by \( x \sim y \). We impose a periodic boundary, deciding that \((0, j)\) is neighbor with \((n-1, j)\) and \((i, 0)\) with \((i, n-1)\), so that the graph becomes a regular 2-dimensional torus. Hence, each vertex of \( V_n \) has exactly 4 neighbors. From now on, the identification \( n \equiv 0 \) holds for all operations on vertices.

A configuration is a mapping from the vertex set \( V_n \) to the state space \( W = \{-1, +1\} \). Their set is denoted by \( \mathcal{X}_n = W^{V_n} \) and called the configuration set. The values of a configuration can be viewed as a coloring of the lattice. Let \( \sigma \) be a configuration. For convenience, we shall retain the following coloring interpretation:

\[
\begin{align*}
\sigma(x) = +1 & \iff \text{vertex } x \text{ is black} \\
\sigma(x) = -1 & \iff \text{vertex } x \text{ is white}
\end{align*}
\]

Here, we shall deal with one of the simplest and most widely studied parametric families of random field distributions: the Ising model (see e.g. Georgii (1988), Malyshev and Minlos (1991)).

**Definition 1.1** Let \( a \) and \( b \) be two reals. The Ising model on the square lattice \( V_n \) with parameters \( a \) and \( b \) is the probability measure \( \mu_{a,b}^n \) on \( \mathcal{X}_n = \{-1, +1\}^{V_n} \) defined by:

\[
\forall \sigma \in \mathcal{X}_n, \quad \mu_{a,b}^n(\sigma) = \frac{1}{Z_{a,b}^n} \exp \left( a \sum_{x \in V_n} \sigma(x) + b \sum_{x \sim y} \sigma(x)\sigma(y) \right),
\]

where the normalizing constant \( Z_{a,b}^n \) is such that \( \sum_{\sigma \in \mathcal{X}_n} \mu_{a,b}^n(\sigma) = 1 \).

In the classical presentation of statistical physics, the elements of \( \mathcal{X}_n \) are spin configurations; each vertex of \( V_n \) is an atom whose spin is either positive or negative. Here, we
shall simply talk about positive or negative vertices instead of positive or negative spins. The parameters $a$ and $b$ are respectively the surface potential and the pair potential. For $a > 0$ (resp. $a < 0$), the measure $\mu_{a,b}^n$ gives a higher weight to configurations with a large number of positive (resp. negative) vertices. The parameter $b$ represents the interaction between vertices: for $b > 0$, the measure $\mu_{a,b}^n$ tends to favor groups of neighboring vertices with the same spin whereas for $b < 0$, a positive vertex will be more likely surrounded by negative neighbors. For $b = 0$, $\mu_{a,0}^n$ is a product measure: all vertices are mutually independent, positive with probability $p = e^a/(e^a + e^{-a})$ or negative with probability $1 - p$. The classical parameter $\beta = 1/T$ which corresponds to the inverse of the temperature is not relevant here and is omitted in (1). Observe that the model remains unchanged by swapping positives and negatives vertices and replacing $a$ by $-a$. Hence, we chose to study negative values of $a$.

As the size $n$ of the lattice tends to infinity, the surface potential $a = a(n)$ is allowed to depend on $n$ whereas the pair potential $b$ remains fixed. We focus on the case $a(n) \to -\infty$ which corresponds to rare positives vertices among a majority of negative ones. Then, in order to describe this situation, the notion of local configuration is introduced. A local configuration concerns a fixed number (not depending on $n$) of vertices and describes a certain set of positive vertices: see Section 2 for a precise definition and Figure 1 for examples. Ganesh et al. (2000) established that the distribution of the number of positive vertices is approximately Poisson provided the surface potential $a(n)$ tends to $-\infty$ and the pair potential $b$ is positive. In Coupier (2005), this result is generalized to any value of $b$ and to any local configuration. It is recalled here in part (i) of Theorem 3.1.

In this paper, we are interested in the occurrence in $V_n$ of local configurations corresponding to 4-connected components of positive vertices (or black vertices in the coloring interpretation). See Figure 1 for an example. These components are known in the combinatorics literature as square lattice animals or polyominoes: see e.g. Klarner (1967). They are defined as connected clusters of squares in the plane. The size of a lattice animal is simply the number of squares forming it. For instance, the “Tetris” game uses all lattice animals of size 4 (see Figure 2).

Part (i) of Theorem 3.1 can be extended to some given families of square lattice animals: it produces the Poisson approximations (ii) and (iii) of Theorem 3.1. A simulation (Figure 4) illustrates these two results and the key role played by the pair potential $b$. Moreover, the Poisson character of the number of copies occurring in $V_n$ of a given lattice animal is tested by a chi-square test.

The problem of estimating the surface and pair potential $a$ and $b$ of an Ising model is of high importance in applications and several techniques have been proposed: see e.g. Younes (1988). The most famous and performant of them is the pseudolikelihood method (see Graffigne (1987)). Using lattice animals, a new estimation algorithm is proposed, derived from Theorem 3.1 and which is relatively easy to implement.

The paper is organized as follows. Section 2 is devoted to the notion of local configuration. The number $k(\eta)$ of positive vertices forming a local configuration $\eta$ and its perimeter $\gamma(\eta)$ will be defined. Thus, the connection with square lattice animals is made. The Poisson approximations are given in Section 3. They are discussed and illustrated. Finally, in Section
4, an algorithm to estimate the two parameters \(a\) and \(b\) of the Ising model of Definition 1.1 is proposed. It will be tested on simulations and its results will be commented.

2 Local configurations and Animals

Let us start with some notations and definitions. As usual, the graph distance \(d\) is defined as the minimal length of a path (with respect to 4-connectivity) between two vertices. We shall denote by \(B(x, r)\) the ball of center \(x\) and radius \(r\):

\[
B(x, r) = \{ y \in V_n ; d(x, y) \leq r \}.
\]

In order to avoid unpleasant situations, like self-overlapping balls, we will always assume that \(n > 2r\). Two properties of the balls \(B(x, r)\) will be crucial in what follows. The first one is that two balls with the same radius are translated of each other: \(B(x+y, r) = y+B(x, r)\). The second one is that for \(n > 2r\), the cardinality of \(B(x, r)\) depends only on \(r\) and not on \(x\) nor \(n\).

Let \(r\) be a positive real, and consider a fixed ball with radius \(r\), say \(B(0, r)\). We denote by \(\mathcal{D}_r = W^{B(0, r)}\) the set of configurations on that ball. They will be called local configurations of radius \(r\). A local configuration \(\eta \in \mathcal{D}_r\) is determined by its subset \(V_+(\eta) \subset B(0, r)\) of positive vertices:

\[
V_+(\eta) = \{ x \in B(0, r), \eta(x) = +1 \}.
\]

The cardinality of this set will be denoted by \(k(\eta)\) and its complementary set in \(B(0, r)\), i.e. the set of negative vertices of \(\eta\), by \(V_-(\eta)\). Of course, there exists only a finite number of local configurations of radius \(r\) (precisely \(2^{|B(0, r)|}\)). The perimeter \(\gamma(\eta)\) of \(\eta\) is defined as follows:

\[
\gamma(\eta) = 4|V_+(\eta)| - 2|\{\{x, y\} \in V_+(\eta) \times V_+(\eta), \; x \sim y\}|.
\]

If the vertices at distance \(r\) of the center \(0\) all belong to \(V_-(\eta)\) (as in Figure 1), \(\gamma(\eta)\) becomes simply

\[
\gamma(\eta) = |\{\{x, y\} \in V_+(\eta) \times V_-(\eta), \; x \sim y\}|.
\]

In this case, it can be interpreted as the number of pairs of neighboring vertices \(x\) and \(y\) of \(B(0, r)\) having opposite spins under \(\eta\). Each element \(\eta\) belonging to \(\mathcal{D}_r\) describes a certain coloring of the ball \(B(0, r)\) made up of \(k(\eta)\) black vertices. Roughly speaking, the perimeter \(\gamma(\eta)\) represents the contour length of the set formed by the black vertices of the coloring \(\eta\).

Let \(\eta \in \mathcal{D}_r\). For each vertex \(x \in V_n\), denote by \(\eta_x\) the translation of \(\eta\) onto the ball \(B(x, r)\) (up to periodic boundary conditions):

\[
\forall y \in V_n, \; d(0, y) \leq r \implies \eta_x(x + y) = \eta(y).
\]

Let us denote by \(I^n_\|\) the indicator function defined on \(\mathcal{X}_n\) as follows: \(I^n_\| (\sigma)\) is 1 if the restriction of the configuration \(\sigma \in \mathcal{X}_n\) to the ball \(B(x, r)\) is \(\eta_x\) and 0 otherwise. Finally,
Figure 1: From left to right: two local configurations $\eta_1$ and $\eta_2$ of the ball $B(0, 3)$ interpreted as colorings, with $k(\eta_1) = 6$, $k(\eta_2) = 4$ black vertices and perimeters $\gamma(\eta_1) = 18$, $\gamma(\eta_2) = 10$. The set $V_+(\eta_2)$ is 4-connected whereas $V_+(\eta_1)$ is not.

Let us define the random variable $X_n(\eta)$ which counts the number of copies of the local configuration $\eta$ in $G_n$: 

$$X_n(\eta) = \sum_{x \in V_n} I^n_x.$$ 

Due to periodicity, this sum bears over $n^2$ indicator functions $I^n_x$, which have the same distribution.

We are interested in the occurrence in the lattice of local configurations whose set of positive (or black) vertices is connected (with respect to 4-connectivity). These 4-connected components are known in the combinatorics literature as square lattice animals: see Klarner (1967). Denote by $A_k$ the set of size $k$ animals and by $a_k$ its cardinality. The integer $a_k$ represents the number of 4-connected components one can make with exactly $k$ squares in the plane (up to translations). Counting them is a difficult combinatorial problem and there is no general expression for $a_k$. However, some asymptotic results are known: in Klarner (1967), a concatenation argument shows that there exists a constant $\alpha$, called growth constant, such that:

$$\lim_{k \to \infty} (a_k)^{1/k} = \sup_{k \geq 1} (a_k)^{1/k} = \alpha .$$

The exact value of $\alpha$ is unknown, numerical estimates give $\alpha \simeq 4.06$ and the best published rigorous bounds for it are $3.9 < \alpha < 4.65$; see Conway and Guttmann (1995), Jensen and Guttmann (2000) and Klarner and Rivest (1973). But thanks to some numerical studies\footnote{for up-to-date informations on the topic, see the web-site of the “On-line Encyclopedia of Integer Sequences”, \url{http://www.research.att.com/~njas/sequences/} and references therein.}, the first values of the sequence $(a_k)_{k \geq 1}$ are known up to $k = 47$.

The two extremes animals of Figure 2 (ii) will be denoted by $A_1$ and $A_2$. Throughout this paper, they will illustrate our remarks and comments.

Let us fix $k > 0$ and a radius $r \geq k$. To each animal of size $k$, a local configuration of the ball $B(0, r)$ will be associated. Let $A \in A_k$. Denote by $D_r(A)$ the subset of $D_r$
formed by the local configurations $\eta$ whose set of positive vertices $V_+(\eta)$ is isomorphic to $A$, in the sense of graph structure. In particular, all elements of $\mathcal{D}_r(A)$ have the same number of positive vertices and the same perimeter. Let us choose one of them, say $\eta_A$, that we shall call the local configuration associated to $A$. Then, the perimeter of the square lattice animal $A$ is naturally defined as the perimeter of its associated local configuration $\eta_A$. For example, the local configuration $\eta_2$ of Figure 1 could be associated to the animal $A_2$ represented on Figure 2.

All animals of size 3 have the same perimeter (Figure 2 (i)). However, this becomes false for $k \geq 4$ (Figure 2 (ii)). Hence, let us denote by $\Gamma_k$ the set of possible perimeters of animals of size $k$. For instance, $\Gamma_3 = \{8\}$ and $\Gamma_4 = \{8, 10\}$. The set of animals of size $k$ and perimeter $\gamma$ will be denoted by $A_{k, \gamma}$ and its cardinality by $a_{k, \gamma}$. Of course, $\sum_{\gamma \in \Gamma_k} a_{k, \gamma} = a_k$. As in the case of the sequence $(a_k)_{k \geq 1}$, only the first values of $\{a_{k, \gamma}, \gamma \in \Gamma_k\}_{k \geq 1}$ are known, which will be enough in practice for the estimation of potentials $a$ and $b$ (see Section 4).

3 Poisson Approximations

Let us define the following random variables:

$$X_n(k, \gamma) = \sum_{A \in A_{k, \gamma}} X_n(\eta_A) \quad \text{and} \quad X_n(k) = \sum_{A \in A_k} X_n(\eta_A) = \sum_{\gamma \in \Gamma_k} X_n(k, \gamma)$$

where, for every animal $A \in A_k$, $\eta_A$ is the associated local configuration. As we shall see below, $X_n(k, \gamma)$ counts the occurrences of animals of size $k$ and perimeter $\gamma$, and $X_n(k)$ counts those of animals of size $k$. Here is the statement of Poisson approximations for the random variables $X_n(\eta)$, $X_n(k, \gamma)$ and $X_n(k)$:

**Theorem 3.1** Let $k \geq 1$, $r \geq k$ be fixed integers and $c > 0$ be a constant. Assume that the pair potential $b \in \mathbb{R}$ is fixed and that the surface potential $a = a(n)$ satisfies:

$$ka(n) = \log \left( \frac{\sqrt{c}}{n} \right).$$

(2)

Let us denote by $\mathcal{P}(\lambda)$ the Poisson distribution with parameter $\lambda$. Let $\eta$ be a local configuration of the ball $B(0, r)$ such that $k(\eta) = k$ and $\gamma$ be an element of $\Gamma_k$. Then, as $n$ tends to infinity:
(i) the distribution of $X_n(\eta)$ converges weakly to $\mathcal{P}(ce^{-2b\gamma(\eta)})$;
(ii) the distribution of $X_n(k, \gamma)$ converges weakly to $\mathcal{P}(ca_{k, \gamma}e^{-2b\gamma})$;
(iii) the distribution of $X_n(k)$ converges weakly to $\mathcal{P}(c\sum_{\gamma \in \Gamma_k} a_{k, \gamma}e^{-2b\gamma})$.

The rest of this section is devoted to comments and illustrations of this result.

- Part (i) is proved in Coupier (2005). It is based on the moment method (see Bollobás (1985), p. 25). In the case $b \geq 0$, a more precise result can be proved: the total variation distance between the probability distribution of $X_n(\eta)$ and the Poisson distribution with parameter $ce^{-2b\gamma(\eta)}$ is of order $n^{-2/b}$.

The proof of part (i) can be extended to the number of copies of some given families of square lattice animals: this produces parts (ii) and (iii) and, in particular, the following limit which will be useful for estimating potentials $a$ and $b$ in the next section:

$$\lim_{n \to +\infty} \mathbf{E}_{\mu_n^a,b}[X_n(k, \gamma)] = ca_{k, \gamma}e^{-2b\gamma},$$

where $\mathbf{E}_{\mu_n^a,b}[.]$ denotes the expectation relative to $\mu_n^a,b$. When the pair potential $b$ is null, parts (ii) and (iii) are particular cases of Theorem 2.4 of Coupier et al. (2005).

- For any given local configuration $\eta$ of radius $r$, the event $X_n(\eta) > 0$ corresponds to the occurrence of $\eta$ in $V_n$. It has been proved in Coupier et al. (2005) that:

$$\text{if } \lim_{n \to +\infty} ne^{a(n)k(\eta)} = 0 \text{ then } \lim_{n \to +\infty} \mu_n^{a,b}(X_n(\eta) > 0) = 0.$$

Then, if the surface potential $a(n)$ satisfies (2), the previous result means that asymptotically there will be no local configuration with (strictly) more than $k$ positive vertices in the lattice. In other words, if $\eta_x$ (with $k(\eta) = k$) occurs on the ball $B(x, r)$ then vertices of $B(x, R) \setminus B(x, r)$, $R \geq r$, have negative vertices with probability tending to 1. This has two immediate consequences. Firstly, the limit distributions of the random variables $X_n(k, \gamma)$ and $X_n(k)$ do not depend on the choice of the associated local configurations $\eta_A$, $A \in \mathcal{A}_k$. Moreover, as $n$ tends to infinity, $X_n(k, \gamma)$ (resp. $X_n(k)$) is almost surely equal to the number of copies of animals of size $k$ and perimeter $\gamma$ (resp. of size $k$) occurring in $V_n$.

- For a large value of $n$ ($n = 900$), the Poisson approximation (ii) will be tested with a chi-square test. For potentials $a = -1.41$ and $b = 0.1$, $K = 500$ realizations of the measure $\mu_n^{a,b}$ are generated. For each of them, the number of copies of the lattice animal $A_1$ of Figure 2 (ii) is computed. Recall that $A_1$ is the only lattice animal with size $k = 4$ and perimeter $\gamma = 8$ ($a_{4,8} = 1$). This produces the sample $\{X_i\}_{i=1,\ldots,K}$, represented by a bar chart in Figure 3. The set of the values taken by the $X_i$’s is $\{0, \ldots, 5\}$. The hypothesis which will be tested is

$$\mathcal{H}_0 : \mathbb{P}(X_i = m) = P_0(m), \forall m = 0, \ldots, 5,$$

where $P_0$ denotes the Poisson distribution with parameter $\lambda = ca_{k, \gamma}e^{-2b\gamma} \approx 2.02$. The constant $c$ satisfies (2) with $a = -1.41$, $k = 4$ and $n = 900$. Let us denote by $\hat{P}$ the
empirical distribution of the sample \( \{X_i\}_{i=1,...,K} \) on \( \{0, \ldots, 5\} \). Then, the \( p \)-value for the chi-square test for the adjustment of \( \hat{P} \) by \( P_0 \) is \( 4.44 \times 10^{-16} \). So, the null hypothesis \( \mathcal{H}_0 \) is strongly rejected.

Thanks to the empirical frequency of the \( X_i \)’s, the estimator \( \hat{\lambda} \) of the maximum likelihood is computed: \( \hat{\lambda} = \sum X_i / K \simeq 1.43 \). This time, with \( P_0 = P(\hat{\lambda}) \), the \( p \)-value for the chi-square test is 0.44.

As a conclusion, the Poisson character of the random variable \( X_n(4, 8) \), i.e. of the number of occurrences of \( A_1 \), is accepted but its (observed) mean is biased: it is smaller than its asymptotic theoretical mean.

\[ \text{Figure 3: A barchart representing } K = 500 \text{ independent realizations of the number of occurrences of } A_1 \text{ with potentials } a = -1.41, b = 0.1 \text{ and a size } n = 900. \]

- Let us point out here the role of the pair potential \( b \) as the size \( n \) of the lattice tends to infinity. Let \( \eta \in \mathcal{D}_r \) with \( k(\eta) > 0 \). Theorem 3.1 assures that the probability (for \( \mu_{a,b}^n \)) of \( \eta \) of occurring in the infinite graph is equal to

\[ 1 - e^{-\kappa e^{-2k\gamma(\eta)}}. \]

So, if \( b > 0 \) (resp. \( b < 0 \)), this probability is a decreasing (resp. increasing) function of the perimeter \( \gamma(\eta) \). In other words, if \( b > 0 \) (resp. \( b < 0 \)), among the local configurations having the same number of positive vertices, those having the highest asymptotic probability of occurring in the lattice \( V_n \) are those having the smallest (resp. largest) perimeter.

Figure 4 shows a simulation where only 2 animals of size 4 occur; \( A_1 \) and \( A_2 \). Recall that \( A_1 \) is the unique animal of size 4 having a perimeter equal to 8 (\( a_{4,8} = 1 \)) and \( A_2 \) is one of the \( a_{4,10} = 18 \) animals of size 4 and perimeter 10. We are going to approximate the probability of occurring of a given animal or of a given family of animals, in the (large) lattice \( V_n \), by their limits (given by Theorem 3.1). Figure 4 is realized with \( a = -0.7 \), \( b = 0.3 \) and \( n = 150 \). So, for a size \( k = 4 \), relation (2) is satisfied for \( c \simeq 83.20 \). Hence, the probability of \( A_1 \) is

\[ 1 - \exp \left( -c \exp(-2 \times b \times 8) \right) \simeq 0.49 \]
and that of any given animal of size 4 and perimeter 10 is

\[ 1 - \exp(-c \exp(-2 \times b \times 10)) \approx 0.19 . \]

So, the animal \( A_2 \) (for instance) had a small probability of occurring in Figure 4. However, the probability for this simulation of containing at least one element of \( A_{4,10} \) is close to 1:

\[ 1 - \exp(-c \times a_{4,10} \exp(-2 \times b \times 10)) \approx 0.98 . \]

Figure 4: A realization of the Ising model of Definition 1.1 with \( a = -0.7, b = 0.3 \) and \( n = 150 \).

4 Application to estimation

Let us start with some words about the simulations. It is possible to obtain exact samples of \( \mu_{a,b}^{n} \) by using the famous “Coupling From The Past” method of Propp and Wilson (1996). This coupling requires that the spin system is attractive, using the vocabulary of Liggett (1985). It is true for positive values of the pair potential \( b \). Furthermore, this algorithm works well if the system is above (and not to close to) the critical temperature: i.e. for \( b < b_c = \log(1 + \sqrt{2})/2 \approx 0.441 \) (see Onsager (1944)). All simulations of this paper have
been realized with Propp and Wilson’s algorithm and for a pair potential $0 \leq b \leq 0.3$.
Now, suppose that we are given a single realization $\sigma$ of the measure $\mu_{a,b}^m$ (with $a < 0$, $b$ as
above and $n$ large). Our goal is to construct some estimators of the two parameters $a$ and
$b$ from this single realization $\sigma$.
Let $m$ be a large integer such that the square of the ratio $\kappa = n/m$ is large too. In practice,
we shall choose $n = 1500$ and $m = 150$ (hence, $\kappa^2 = 100$). Then the lattice $V_n$ is divided
into $\kappa^2$ subsets of vertices of size $m$. Denote by $\sigma_1, \ldots, \sigma_{\kappa^2}$ the restrictions of the realization
$\sigma$ to each of these subsets. If $(\sigma_1, \ldots, \sigma_{\kappa^2})$ was a sample of $\mu_{a,b}^m$, then the empirical mean
$\kappa^{-2} \sum_{i=1}^{\kappa^2} X_m(k, \gamma)(\sigma_i)$ would be close to the expected number $E_{a,b}[X_m(k, \gamma)]$ of copies
of animals of size $k$ and perimeter $\gamma$ occurring in a realization of $\mu_{a,b}^m$. Of course, the
hypothesis of independence between the $\sigma_i$’s is false. However, in their famous article,
Dobrushin and Shlosman (1985) proved the exponential decay of correlations provided
the surface potential $|a|$ is sufficiently large. This corresponds exactly to our context and
justifies that the $\sigma_i$’s can be considered as independent realizations of $\mu_{a,b}^m$.

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<td>-</td>
<td>0</td>
<td>0</td>
<td>0.01</td>
<td>0.01</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 1: A realization $\sigma$ of $\mu_{a,b}^m$ is generated with $n = 1500$, $a = -1$ and $b = 0.1$. This array
represents the empirical means of all animals occurring in the sub-realizations $\sigma_1, \ldots, \sigma_{100}$
(of size $m = 150$), according to their size and their perimeter. The symbol “-” means there
is no animal corresponding to such size and such perimeter.

For all size $k$, let us define $c_{k,m} > 0$ such that $ka = \log(\sqrt{c_{k,m}/m})$. It has been shown in
the previous section that $E_{a,b}[X_m(k, \gamma)]$ is approximately equal to $c_{k,m}a_k \gamma e^{-2\gamma}$ provided
the size $m$ of the lattice is large enough. Let $k' \geq k$. The following equalities

$$\log \left( \frac{\sqrt{c_{k',m}}}{m} \right) = k'a = ka + (k' - k)a = \log \left( \frac{\sqrt{c_{k,m}e^{2a(k'-k)}}}{m} \right)$$

imply $c_{k',m} = c_{k,m} e^{2a(k'-k)}$. Hence, for $\gamma' \in \Gamma_{k'}$ and $\gamma \in \Gamma_k$, the ratio

$$\frac{a_{k,\gamma} \times E_{a,b}[X_m(k', \gamma')]}{a_{k',\gamma'} \times E_{a,b}[X_m(k, \gamma)]}$$

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is approximately equal to $e^{2a(k'-k)+2b(\gamma-\gamma')}$ (the constant $c_{k,m}$ disappears). Finally, assuming that $(\sigma_1, \ldots, \sigma_{\kappa^2})$ is a sample of $\mu_{a,b}^n$, the quantity $\theta(k, k'; \gamma, \gamma')$ defined by

$$\theta(k, k'; \gamma, \gamma') = \frac{1}{2} \log \left( \frac{a_{k,\gamma} \times \sum_{i=1}^{\kappa^2} X_m(k', \gamma')(\sigma_i)}{a_{k',\gamma'} \times \sum_{i=1}^{\kappa^2} X_m(k, \gamma)(\sigma_i)} \right)$$

is close to $a(k' - k) + b(\gamma - \gamma')$. In particular, for $k \geq 1$ and $\gamma, \gamma + 2 \in \Gamma_k$, $\theta(k, k+1; \gamma, \gamma+2)$ and $\theta(k, k; \gamma, \gamma+2)$ estimate respectively the quantities $a - 2b$ and $-2b$. For example, thanks to the data of Table 1,

$$\theta(3, 4; 8, 10) = \frac{1}{2} \log \left( \frac{6 \times 8.3}{18 \times 34.18} \right) \simeq -1.257 \quad \text{and}$$

$$\theta(4, 4; 8, 10) = \frac{1}{2} \log \left( \frac{1 \times 8.3}{18 \times 0.69} \right) \simeq -0.202$$

which are indeed close to $a - 2b = -1.2$ and $-2b = -0.2$.

Moreover, it seems that the convergence of $X_m(k, \gamma)$ to $\mathcal{P}(c_{k,m} a_{k,\gamma} e^{-2b\gamma})$ becomes slow as the size $k$ increases. It is the reason why we focus on animals of size $k \leq 6$. Precisely, the estimators $\tilde{b}(\sigma)$ and $\tilde{a}(\sigma)$ of the pair potential $b$ and the surface potential $a$ are defined by:

$$\tilde{b}(\sigma) = -\frac{1}{2} \times 3 (\theta(4, 4; 8, 10) + \theta(5, 5; 10, 12) + \theta(6, 6; 12, 14)) \quad \text{and}$$

$$\tilde{a}(\sigma) = \frac{1}{5} (\theta(1, 2; 4, 6) + \theta(2, 3; 6, 8) + \theta(3, 4; 8, 10) + \theta(4, 5; 10, 12) + \theta(5, 6; 12, 14)) \times 2 \tilde{b}(\sigma)$$

In order to evaluate our estimation of potentials $a$ and $b$, we imlemented the following algorithm:

1. An exact realization $\sigma$ of $\mu_{a,b}^n$ is generated and it is “divided” into $\kappa^2 = (n/m)^2$ sub-realizations $\sigma_1, \ldots, \sigma_{\kappa^2}$ of size $m$.

2. For each $k$ and each $\gamma \in \Gamma_k$, the animals of size $k$ and perimeter $\gamma$ occurring in $\sigma_i$ are enumerated for $i = 1, \ldots, \kappa^2$ and the empirical means $\kappa^{-2} \sum_{i=1}^{\kappa^2} X_m(k, \gamma)(\sigma_i)$ are computed.

3. The estimators $\tilde{b}(\sigma)$ and $\tilde{a}(\sigma)$ are computed.

The estimators of the realization $\sigma$ of Table 1 are: $\tilde{a}(\sigma) = -1.063$ and $\tilde{b}(\sigma) = 0.119$. Our Poisson approximations (Theorem 3.1) are valid for fixed value of the pair potential $b$ and a surface potential $a$ which tends to $-\infty$. Consequently, in practice, potentials $a$ and $b$ are chosen so that the ratio $|a|/b$ remains “large”. Experimental results are presented in Table 2.

The Poisson approximation of $X_m(k, \gamma)$ is valid as soon as the surface potential $a = a(m)$ satisfies $ka(m) = \log(\sqrt{c}/m)$. Now, the algorithm above consists in adjusting the constant $c = c_{k,m}$ to each size $k$ of animals in order to have the identity $ka = \log(\sqrt{c_{k,m}}/m)$
<table>
<thead>
<tr>
<th>Potentials</th>
<th>Estimators</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a = -0.8$</td>
<td>$\hat{a}(\sigma) = -0.893$ $\hat{b}(\sigma) = 0.085$</td>
</tr>
<tr>
<td>$a = -1$</td>
<td>$\hat{a}(\sigma) = -1.062$ $\hat{b}(\sigma) = 0.157$</td>
</tr>
<tr>
<td>$a = -1.2$</td>
<td>$\hat{a}(\sigma) = -1.241$ $\hat{b}(\sigma) = 0.171$</td>
</tr>
<tr>
<td>$a = -1.2$</td>
<td>$\hat{a}(\sigma) = -0.678$ $\hat{b}(\sigma) = 0.504$</td>
</tr>
</tbody>
</table>

Table 2: For each value of $(a, b)$, a realization $\sigma$ of the measure $\mu_{a,b}$ is generated. This array contains the corresponding estimators $\hat{a}(\sigma)$ and $\hat{b}(\sigma)$.

and the corresponding Poisson approximation. This adjustment of the constant $c$ produces a limited efficiency of our method and of our experimental results (Table 2).

Finally, recall that the pair potential $b$ controls the degree of local dependence between vertices. As a consequence, the hypothesis of independence between the $\sigma_i$’s becomes questionable as $b$ increases. This explains the bad estimation of the couple $(a, b) = (-1.2, 0.25)$ in Table 2.

Acknowledgments

We would like to thank Tony Guttmann for making the numbers $a_{k,\gamma}$ of animals of size $k$ and perimeter $\gamma$ available to us. Without these numbers, no estimation is possible.

References


