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GIBBS RANDOM FIELDS: TEMPERATURE AND PARAMETER ANALYSIS *

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Abstract

Gibbs random field (GRF) models work well for synthesizing complex natural-looking image data with a small number of parameters; however, estimation methods for these parameters have a lot of problems. This paper addresses the analysis problem in a new way by examining the role of the temperature parameter of the Gibbs distribution. Studies of the model energy with respect to the temperature are used to indicate pattern equilibrium and regions of different behavior, analogous to the existence of distinct phases in a physical system. The results on equilibrium and regions of different "phases" are offered as explanations for some of the peculiar behavior of current estimation algorithms.

1 Gibbs random fields

This paper focuses on the discrete Gibbs random field (GRF), defined as follows. Let an image be represented by a finite rectangular $M \times N$ lattice $\mathcal{S}$ with a neighborhood structure $\mathbf{N} = \{\mathcal{N}_s, s \in \mathcal{S}\}$ where $\mathcal{N}_s \subseteq \mathcal{S}$ is the set of sites which are neighbors of the site $s \in \mathcal{S}$. Every site has a graylevel value $x_s \in \Lambda = \{0, 1, \ldots, n-1\}$. Let $\mathbf{x}$ be the vector $(x_s, 1 \leq s \leq |\mathcal{S}|)$ of site graylevel values and Ω be the set of all configurations taken by $\mathbf{x}$. A neighborhood structure is said to be *symmetric* if $\forall s, r \in \mathcal{S}$, $s \in \mathcal{N}_r$ if and only if $r \in \mathcal{N}_s$.

For the finite periodic lattice $\mathcal{S}$ with a symmetric neighborhood structure, one can define a Gibbs energy. There are many ways to define the energy; the choice studied here is the *auto-binomial* energy of [1], which has been shown to synthesize a variety of natural looking image textures [2]. The homogeneous auto-binomial energy is

$$E(\mathbf{x}) = -\sum_{s \in \mathcal{S}} \left(\alpha x_s + \sum_{r \in \mathcal{N}_s} \beta_r x_s x_r \right), \qquad (1)$$

where the model parameters are α, the *external field*, and β_r, the bonding interactions. A joint probability distribution is assigned to the Gibbs energy yielding the *Gibbs random field*,

$$P(\mathbf{x}) = \frac{1}{Z} \exp\left(-\frac{1}{T} E(\mathbf{x})\right), \qquad (2)$$

where Z is a positive normalizing constant known in the physics literature as a *partition function* and T is the "temperature" of the field.

The synthesis process is one of finding the configuration in Ω which maximizes the probability $P(\mathbf{x})$, minimizing the Gibbs energy. Image data is typically synthesized iteratively, using a Monte Carlo method such as the Metropolis exchange algorithm. In this algorithm it can be shown that the external field cancels, leaving only the bonding parameters.

If the temperature T is lowered during the Monte Carlo synthesis then the synthesis process becomes an example of *simulated annealing.* Simulated annealing is a popular nonlinear optimization technique where a cost function is substituted for $E(\mathbf{x})$, and consequently minimized. There is a key observation in the simulated annealing literature that prompts the study of temperature presented in this paper. Kirkpatrick, *et. al.*[3] observed that "more optimization" occurs at certain temperatures than at others. These favored temperatures are analogous to the physical idea of a "critical temperature," a point that marks transition between different "phases" of the data.

The reason for considering these physical analogies is that they have important implications for parameter estimation. In this paper the basic temperature behavior of the isotropic auto-binomial GRF is developed. It is shown how this behavior can be used for parameter estimation by combining it with an earlier result relating co-occurrence matrices (pairwise graylevel statistics) to GRF's.

2 Why temperature analysis?

Of course, for the Gibbs random field to be of general use, one needs to be able to estimate its parameters reliably. This is currently not the case. Methods for estimating Gaussian random field models seem to be fairly well studied [4]; methods for general GRF's such as the auto-binomial model have many problems, and their behavior has not been clearly accounted for.

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The popular analysis method of "Besag Codings" [2] involves a maximum likelihood estimator formed over disjoint subsets of the lattice. This nonlinear method is generally considered cumbersome and difficult to use reliably [5]. Even though it is easy to formulate the estimator for the auto-binomial model [6], we confirmed that its performance varies widely for different data – it works well for selected images, but poorly for others. In the next section we propose two new explanations for the variation in performance.

A variety of other estimation methods have been proposed [5, 7] all of which ultimately involve computing counts of blocks in the image having particular graylevel configurations, and then taking logs of ratios of these counts. (Note: the Besag Coding method can also be implemented in this way; we call this the "contingency table" implementation later.) The problem that has been noticed with all of these methods is that often some of the counts are zero, and then one must propose seemingly ad hoc alternatives to avoid log(0) and division by zero. Some of these alternatives have been concluded to work well; however, no one has yet proposed the ranges where they work well, or why. The temperature characterization presented in the next section offers an explanation of these ranges.

In their overview paper, Dubes and Jain [7] review four estimation methods from the literature and discuss some of the shortcomings of the methods. In their conclusions, they raise several questions which they consider outstanding problems in Markov/Gibbs modeling. Two of them are addressed in the rest of this paper. The first is "what regions of the parameter space lead to valid models?" and the second is "what regions in the parameter space put the process into phase transition?"

3 Temperature and energy

Temperature and energy are two physical quantities that turn out to be important for even the simplest GRF estimation. From [8] we know that a given set of GRF parameters will synthesize a variety of texture patterns while its energy is being minimized. This poses an obvious problem – which pattern gets associated with the parameters? One "physical" approach to this is to consider that the pattern is not in "equilibrium" unless its energy has decreased to some level where it has stopped changing. One then associates the model's parameters with the equilibrium pattern. Early experiments assumed the number of iterations required for equilibrium to be on the order of 10-100 [2, 9]. Later we showed that the number of iterations grows with model order and number of graylevels, and can be tens of 1000's in some "practical" cases.

Consider the simplest case, an isotropic first order GRF having $\beta_r = \beta = 1$ with $\mathcal{N}$ consisting of the four nearest neighbors. Nine samples of this GRF are shown in Figure 1 where $N = M = 64$ and $n = 32$ graylevels. Each column corresponds to synthesizing at a different temperature: $T = 1000, 100, .01$ from left to right. Note that parameters could also be considered as $\beta/T = .001, .01, 100$. From top to bottom the samples represent "snapshots" at $i = 10$, 100, and 1000 iterations during the synthesis algorithm. Notice that the pattern in the first column does not change; in contrast, the "colder" pattern at the right is still changing after 1000 iterations.

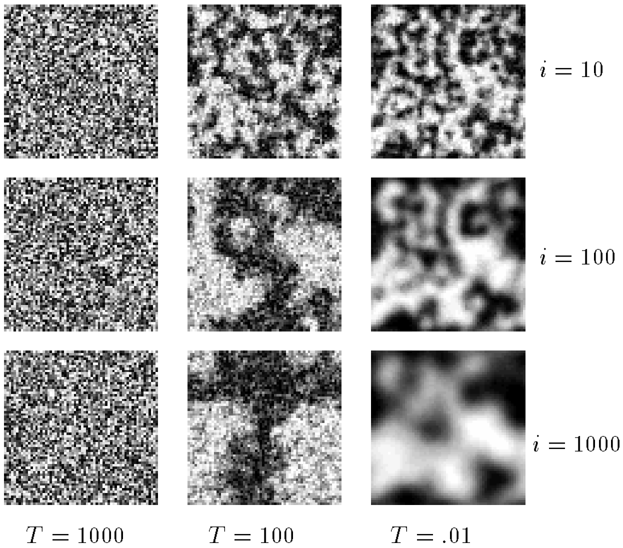

Figure 1: Equilibrium behavior is reached after 10 iterations for $T = 1000$, and after 100 and 1000 iterations for $T = 100, T = .01$, respectively.

The allowance of 100 iterations for equilibrium corresponds to the middle row of samples for the temperatures shown. When β/T is estimated for samples such as in Figure 1, it will be accurate for the first two columns, but too low for the third column. We offer this explanation for the applications of [6] where they noticed that the parameter estimates needed to be adjusted upward, but did not know why.

Thus, we propose that the first problem with the way estimation methods have been evaluated has to do with a lack of attention to the pattern's equilibrium. An estimate taken while a pattern's energy is still decreasing should not be expected to fit the parameters which are synthesizing the pattern.

As mentioned in the previous section, another problem with the current parameter estimation methods is determining their region of validity. This problem can also be more clearly understood by examining the energy of the GRF at different temperatures. For the GRF shown in Figure 1, the mean energy was computed over 40,000 iterations after an equilibrium time of

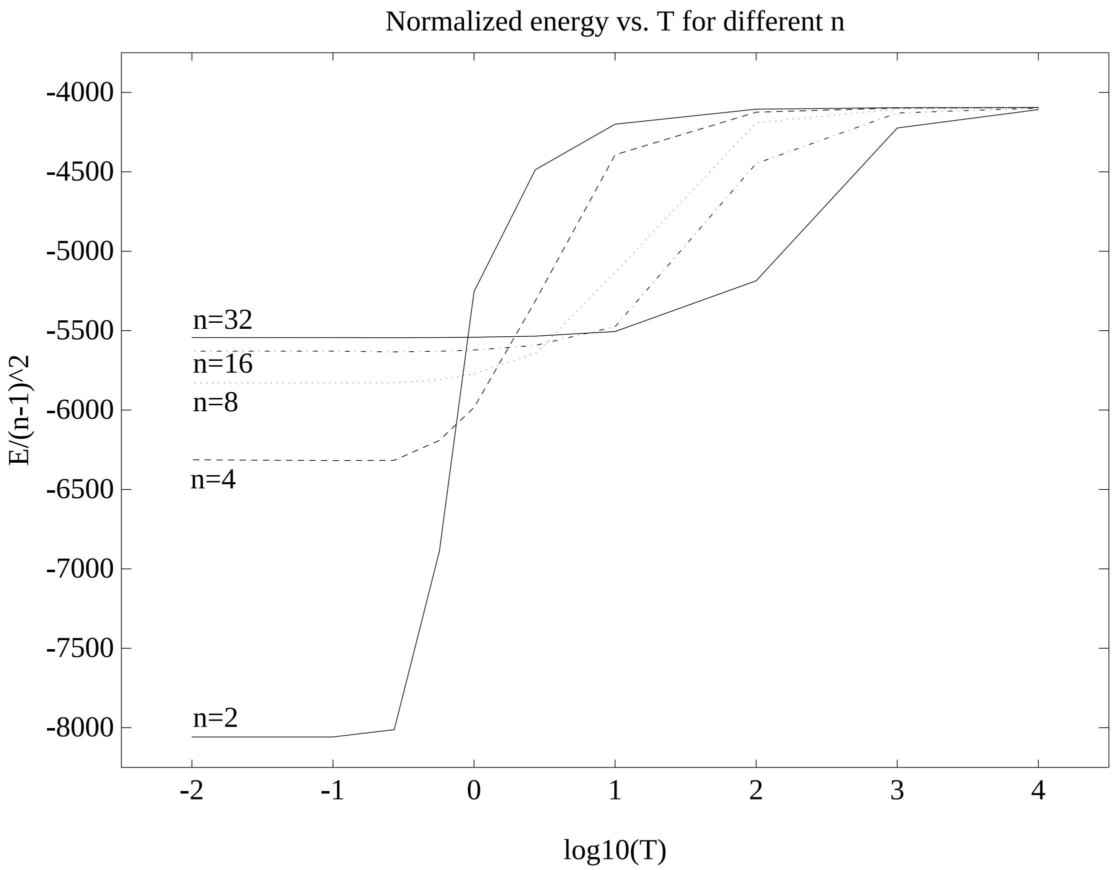

Figure 2: Normalized mean energy at each temperature for five different graylevels, n.

10,000 iterations (excessive for low n but not for high n). The average energy is shown for $\beta = 1$ and $n = 2, 4, 8, 16, 32$ graylevels in Figure 2. All the values are normalized by $(n-1)^2$ so that they align at the high temperature side of the graph. Now, let us consider how this graph illustrates the range of valid parameters β/T for the isotropic first order GRF.

Consider the plot for the GRF when $n = 2$. Notice that at the right all values for $T > 100$ map to the same energy. A similar saturation occurs at the left for cold temperature. Thus, parameters estimated in these plateau regions will not be unique. In fact, the patterns corresponding to the energy at the right are binary noise, and to the energy at the left are images with white on one half and black on the other. If one thinks of the binary image as being composed of a black fluid and a white fluid, it has "mixed" on the right, and "separated" on the left.

Alternatively, one could think of the mixture as being in its liquid state on the right, and frozen into a solid state on the left. Either way, a transition in "phase" of the material occurs in the center. In the center, where the energy changes abruptly as in a true "phase transition," one finds patterns that appear to be generally closer to natural textures.

Although a true "critical temperature" does not exist in this region, we have shown in earlier work that a similar kind of point, which we call a "transition" temperature, T_*, does occur [8]. By measuring the specific heat of the binary process it can be shown to correspond to the same region where the "most optimization" occurs in simulated annealing [3]. For GRF analysis, this region is where the energy fluctuation peaks, and where small changes in the parameters become more significant. In [8] the transition temperature for $n = 2$ was estimated to be at $1/T_* = 1.7$.

This analysis suggests that attempts to estimate parameters should take into account these transition regions and surrounding plateaus. After conducting a brief empirical study of 54 synthetic isotropic "equilibrium" binary GRF textures having parameters $|\beta/T| \in \{.01, .1, .5, .67, 1, 1.25, 1.76, 5, 10\}$, we found that both implementations of the Besag Coding method (one with Newton-Raphson, and one with the contingency tables) performed best over the central range of temperature values, $|\beta/T| \in \{.5, .67, 1, 1.25\}$, just under the estimated $1/T_*$.

A much larger study should be conducted before the accuracy can be meaningfully assessed.

The second explanation promised in this section concerns the missing configurations. From earlier results [8], we know that the GRF energy can be written as a linear combination of co-occurrences. We also know that the co-occurrence matrices will develop structure that indicates which configurations occur with zero probability [10]. Thus, the co-occurrence matrices can be used to determine regions where the positivity condition of the GRF is violated. The co-occurrences also determine the energy, which in turn determines the temperature. For $n > 2$ the lack of certain configurations actually becomes helpful for determining β/T.

These results suggest the following method. During synthesis, one can use the co-occurrence statistics to determine whether or not the energy is still changing. Once the energy has stopped changing, its value can be used to index into the appropriate plot of Figure 2. Alternatively, one can find the corresponding temperature analytically by fitting a sigmoid to each plot, $E_n(T) = \frac{1}{1+cT^{\alpha}}$. The parameters α and c are determined in advance for each curve, and can be used with the co-occurrences to recover T.

For example, when $n = 2$ and the image is 64×64 as in Figure 2, a good approximation is $-E_2(T)/8192 = \frac{.48}{1+T^{4.707}} + .5$. As $T \rightarrow 0$ (freezing), the co-occurrence matrix becomes as diagonal as allowed, with diagonal elements of .98. As $T \rightarrow \infty$ (melting), the co-occurrence matrix becomes uniform, with elements of .5.

4 Summary

The effects of temperature have been characterized for the isotropic auto-binomial Gibbs energy. These results indicate the importance of considering equilibrium and transition behavior when estimating the GRF parameters.

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