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Cluster update algorithm and recognition

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We present a fast and robust cluster update algorithm that is especially efficient in implementing the task of image segmentation using the method of superparamagnetic clustering. We apply it to a Potts model with spin interactions that are are defined by gray-scale differences within the image. Motivated by biological systems, we introduce the concept of neural inhibition to the Potts model realization of the segmentation problem. Including the inhibition term in the Hamiltonian results in enhanced contrast and thereby significantly improves segmentation quality. As a second benefit we can, after equilibration, directly identify the image segments as the clusters formed by the clustering algorithm. To construct a subsequent spin configuration the algorithm performs the standard steps of (i) forming clusters and of (ii) updating the spins in a cluster simultaneously. As opposed to standard algorithms, however, we share the interaction energy between the two steps. Thus, the update probabilities are not independent of the interaction energies. As a consequence, we observe an acceleration of the relaxation by a factor of 10 compared to the Swendson and Wang [Phys. Rev. Lett. **58**, 86 (1987)] procedure.

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The segmentation of images into connected areas or objects is a formidable task and an important step in the process of recognition. Nature provides us with many examples of biological systems that solve this and other tasks related to the recognition problem in highly efficient ways. Taken as such, the problem is ill-defined: one will distinguish different numbers of objects in a noisy picture depending on the level of contrast and resolution. A physicist's answer to the problem has been presented by the method of ''superparamagnetic clustering of data'' [1,2], where the pixels of an image are represented by a Potts model of spins which interact in such a way that neighboring spins corresponding to similar pixels tend to align. Then the image segments (or objects) may be identified as subsets or clusters of correlated spins at a given temperature. At high temperature one will find a disordered paramagnetic phase while, when lowering the temperature, superparamagnetic phases occur with clusters of aligned spins.

From a theoretical point of view any method of simulating a given spin system is equivalent as long as it preserves general concepts such as detailed balance. For practical purposes it is of course desirable to choose a method that is efficient and best adapted to the model. Cluster update algorithms are commonly used to to accelerate the equilibration of large spin systems [3–5]. As opposed to single spin updates following a Metropolis procedure, these algorithms provide a method to update connected clusters of aligned spins simultaneously.

Our approach to the problem is twofold: On the one hand we introduce to the spin model the concept of (i) *global inhibition*, motivated by the analogy to neural visual systems [6], on the other hand (ii) we have developed a cluster algorithm that utilizes the energy landscape, which underlies the equilibration process, in a more efficient way.

(i) The concept of global inhibition is found in many biological neural networks and has successfully been applied also in neural computation [7]. We implement it by adding a small global penalty for spins to align. It serves to identify different clusters by different spin labels without the need to observe the spin correlations over a longer time period.

(ii) In a cluster update algorithm the clusters are formed by ''freezing'' bonds between aligned spins with some probability. Commonly the clusters are then updated independently. We update the clusters taking into account also the interactions on bonds that were not frozen. In addition the inner surface of the larger clusters is reduced by incorporating islands that they might contain. Both of our improvements are implemented while preserving detailed balance. As a result, we observe a significant increase in quality and speed.

Without loss of generality in the following we will use the problem of segmenting an image into individual objects as an example to describe our approach. Specifically, given a picture in form of color (or gray-scale) values $g_1, \ldots, g_N$ on the N sites of a finite two-dimensional (2D) lattice, we have the clustering problem: find ''objects'' i.e., clusters of almost the same color.

We define for each pair of nearest neighbors or *bond* (i,j) on the lattice the distance $\Delta_{ij}=|g_i-g_j|$ and the mean distance $\overline{\Delta}_{ij}$ averaged over all bonds.

To perform the clustering task we assign a spin variable σ_i to each site i and for each bond (i,j) an interaction strength

$$J_{ij}=1-\Delta_{ij}/\overline{\Delta}_{ij}. \tag{1}$$

With the normalization in Eq. (1) the color of sites i,j is assumed to be similar when the gray value distance Δ_{ij} is smaller than the average. Then the interaction strength is positive with a maximum value of 1 for equal color. We implement the spin model in such a way that for neighboring sites with similar color the spins have the tendency to align. For this purpose we use a q-state Potts model with the Hamiltonian

$$H=-\sum_{\langle i,j\rangle} J_{ij}\delta_{\sigma_i\sigma_j}+\frac{\kappa}{N}\sum_{i,j}\ \delta_{\sigma_i\sigma_j}. \tag{2}$$

Here, $\langle i,j\rangle$ denotes that i,j are nearest neighbors connected by a bond (i,j) and δ_{ij} is the Kronecker δ function. The second term is introduced in analogy to neural systems, where it is generally called ''global inhibition.'' It serves to favor different spin values for spins in different clusters, as explained below. This is a concept realized in many neural systems that perform recognition tasks. The segmentation problem is then solved by finding clusters of correlated spins in the low temperature equilibrium states of the Hamiltonian H.

We perform this task by implementing a clustering algorithm: In a first step the ''satisfied'' bonds, i.e., those that connect nearest neighbor pairs of identical spins $\sigma_i=\sigma_j$, are identified. The satisfied bonds (i,j) are then ''frozen'' with some probability p_{ij}.

Sites connected by frozen bonds define the clusters. Each cluster is then updated by assigning to all spins inside the cluster the same new value. Commonly this is done independently for each cluster [3]. In that sense the external bonds connecting the clusters are ''deleted.'' Here, we use a more general cluster algorithm. When choosing a new spin configuration we take these bonds into account. To preserve detailed balance, we adjust the bond freezing probabilities p_{ij} and the interaction on the external bonds.

Our cluster update algorithm, which we call energy-sharing cluster update (ECU) is divided in two basic steps. Similar to the Swendson and Wang cluster algorithm [3], also in our approach the temperature remains fixed and no annealing takes place between the iterations.

(1a) As for any cluster update we first identify the *satisfied* bonds (i,j) with $\sigma_i=\sigma_j$ and freeze these with probability

$$p_{ij}^{(1)}=1-e^{-\beta q_{ij}^{(1)}E_{ij}},$$

when $J_{i,j}>0$ and $E_{ij}=J_{ij}\delta_{\sigma_i\sigma_j}$. Here $1/\beta=k_BT$ is the product of the Boltzmann constant k_B and temperature T.

The additional coefficients

$$q_{ij}^{(1)}=\begin{cases}\alpha^{(1)} & \text{if } (i,j) \text{ is a bond}\\ 0 & \text{else}\end{cases}$$

with $\alpha^{(1)}\leqslant 1$ allow us to ''share'' the interaction energy with the following additional steps. If one chooses $\alpha^{(1)}=1$, then one obtains the usual Swendson-Wang clusters, which may then be updated independently.

(1b) In an intermediate step we identify ''invisible'' islands, i.e., clusters according to step (1a) that have a boundary only with *one* other cluster and have the same spin value. These islands often delay the spin flip of the larger cluster in step (2) as their total boundary may be large. For this reason we want to remove them with some finite probability. This step is not indispensable for our algorithm but it further improves its performance. We freeze the bonds between an island and the surrounding cluster with probability

$$p_{ij}^{(2)}=1-e^{-\beta q_{ij}^{(2)}E_{ij}},$$

where $q_{ij}^{(2)}=\alpha^{(2)}$ if (i,j) is a bond connecting an island with a surrounding cluster after step (1) and otherwise $q_{ij}^{(2)}=0$. We impose the condition $\alpha^{(1)}+\alpha^{(2)}\leqslant 1$. Note that we do not increase the bond freezing probability beyond the Swendson-Wang probability and no size limit for the islands is implied.

(2) Finally we identify the clusters $c_1, \ldots, c_k$ of spins connected by frozen bonds after steps (1a) and (1b). On this system of clusters that in similar approaches is referred to as a hyperlattice [8] we perform a Metropolis update that updates all spins in each cluster simultaneously to a common new label. The Metropolis rate is calculated using the modified Hamiltonian

$$\tilde{H}(\sigma)=-\sum_{\langle i,j\rangle} q_{ij}^{(0)}J_{i,j}\delta_{\sigma_i\sigma_j}+\frac{\kappa}{N}\sum_{i,j}\ \delta_{\sigma_i\sigma_j}. \tag{3}$$

As has been shown on general grounds in [9] detailed balance is preserved under the condition that in the modified Hamiltonian one uses $q_{ij}^{(0)}+q_{ij}^{(1)}+q_{ij}^{(2)}=1$. This amounts to sharing the interaction energy between the clustering and updating steps. Note that the inhibition term in Eq. (3) does not enter the bond freezing probabilities. For the cluster update it has the effect of favoring a different spin value for each cluster.

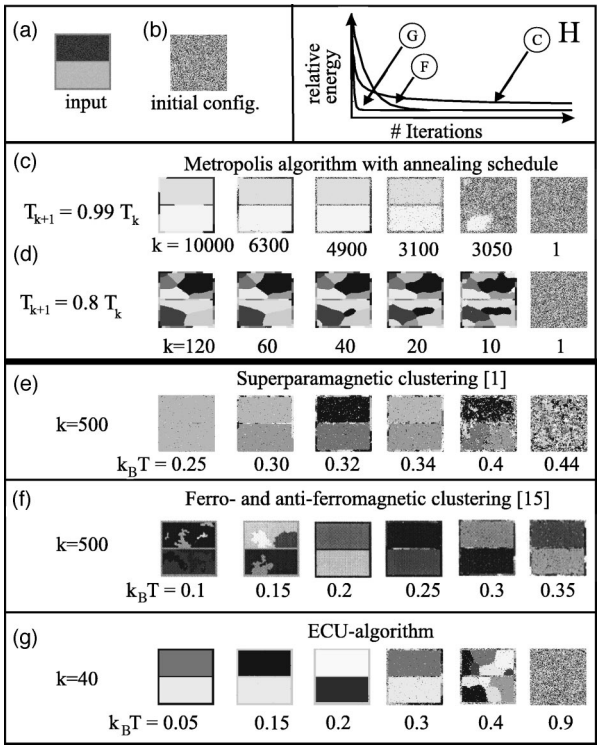

FIG. 1. Comparison of different segmentation methods. As parameters we use $N=128\times128$ and $q=10$ (states of the Potts model). (a) The input image for all simulations consists of two rectangles with gray values $g_i^0=72,152$ and a one pixel thin line surrounding them with $g_i^0=112$. Noise is added $g_i=g_i^0+\xi_i$ that is equally distributed: $\xi_i=-12..12$. (b) The initial random configuration. (c) and (d) Configurations of a local update algorithm (Metropolis: ''Gibbs-Sampler'') at different iterations. (e) Configurations of the SW cluster update algorithm. (f) Configurations of the SW cluster update using antiferromagnetic clustering. (g) Configurations of the ECU-algorithm including inhibition $\kappa=0.2$. (h) The relative energy of the spin-lattice as a function of the number of iteration steps for the different algorithms in (c), (f), and (g) at $k_BT=0.2$.

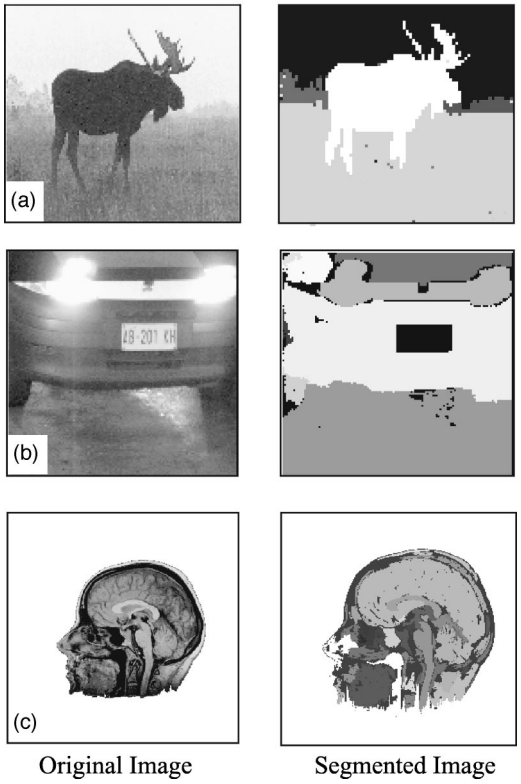

FIG. 2. Applications of the ECU segmentation method. For each picture (a)–(c) the input image and the segmention result of the q-state Potts model after k iterations is shown. (b) shows an intermediate, (a) and (c) show the final result of segmentation after equilibration. (a) Moose in the morning fog. $q=10$, $k=40$. (b) Front of a car. The task is to identify the license plate. $q=10$, $k=12$. (c) NMR-image of the human brain. $q=20$, $k=65$.

We have tested the performance of the proposed segmentation method based on the Hamiltonian H in Eq. (2) with a finite inhibition of $\kappa=0.2$ in combination with the ECU cluster update algorithm with energy sharing parameters $\alpha^{(1)}=\alpha^{(2)}=0.5$. In our experience the efficiency of the algorithm does not depend sensitively on these parameters. Further refinements may be added to improve the segmentation delivered by the ECU algorithm to cope with more delicate recognition problems [10]. We have compared the algorithm to the performance of other known segmentation methods. As methods of reference we have used in particular the method of simulated annealing and the method of superparamagnetic clustering [1] without inhibition ($\kappa=0$) using the standard Swendson and Wang (SW) update. In addition we have tested a variant of the SW update that allows to freeze antiferromagnetic bonds (i,j) when $J_{ij}<0$.

An example that illustrates the different solutions to the segmentation problem is shown in Fig. 1. Let us explain this comparison in some detail. The gray scale values that define the interactions J_{ij} according to Eq. (1) are taken from Fig. 1(a). Some noise is included in this input. All segmentation methods that we consider use $q=10$ state spin variables $\sigma_i=1,\ldots,10$. A random initial configuration of the spins is shown in terms of a gray scale picture in Fig. 1(b). As a first reference we show the sequence of a simulated annealing procedure in Figs. 1(c) and 1(d). Here, the Hamiltonian H in Eq. (2) with $\kappa=0$ is used to define the Metropolis rate of local spin updates [11,12]. After each sweep of N spin updates the temperature is lowered by a constant factor λ [13]. We started with a temperature $k_BT_0=1.0$ and lowered by $\lambda=0.999\,92$ in Fig. 1(c) and $\lambda=0.8$ in Fig. 1(d) for each sweep. The spin configurations at intermediate steps are shown in Figs. 1(c) and 1(d). In the slower annealing procedure the two large rectangles in the image are segmented according to the original picture, while the finer structure is not recognized by this algorithm. When the faster schedule is applied as in Fig. 1(d) then even the larger connected areas are divided into artificial segments. Obviously the simulated annealing method is inefficient for the segmentation task and due to slowing down at low temperatures the local update is very time consuming. Even optimizing the annealing rate during the schedule cannot change this picture as an extremely slow rate is needed to indentify the fine structure of the thin border line.

In Figs. 1(e)–1(g) we compare different cluster update algorithms that avoid the problem of slowing down and we test the influence of the inhibition term and the energy sharing that are included only in Fig. 1(g). Comparing the series of spin configurations in Figs. 1(e) and 1(g) one notices that

the inhibition term in Fig. 1(g) indeed introduces a forced contrast between different segments as compared to 1(e), in particular at $k_BT=0.25$ and $k_BT=0.2$. Also the increase in speed is remarkable.

In Fig. 1(f) we test a cluster update algorithm [14,15] that includes antiferromagnetic clustering where in the clustering step (1a) antiferromagnetic bonds with $J_{ij}<0$ and $\sigma_i \neq \sigma_j$ are frozen with probability $p_{ij}=1-\exp[\beta J_{ij}]$. The clusters defined by ferro- and antiferromagnetic bonds are updated while preserving $\sigma_i=\sigma_j$ on the ferromagnetic and $\sigma_i \neq \sigma_j$ on the antiferromagnetic bonds. This method introduces additional contrast between areas of different input color, but it fails at low temperature where artifacts are generated due to the noise in the input. The convergence characteristic of the different algorithms is shown in Fig. 1(h), where the energy of the spin-lattice is plotted as a function of time at fixed temperature. The relaxation time of the ECU-algorithm is about ten times faster than that of the other algorithms.

Let us note that the only parameters that enter our segmentation method are the factors of proportionality $\alpha^{(1)},\alpha^{(2)}$ that determine the share of energy for the bond freezing steps and the inhibition strength κ. Mainly the α-parameters are relevant for the efficiency of the segmentation, while κ indroduces some contrast to the representation of the clusters in terms of spin values. We have not attempted to optimize the choice of the parameters to speed the segmentation of Fig. 1(a). Rather, we are interested in a general purpose algorithm and we have successfully tested the robustness of the ECU segmentation with the present choice of parameters for many different pictures. To demonstrate this robustness we show three examples in Fig. 2. Despite the bad quality of the input a usable segmentation was found within a small number of iterations. A seemingly continuous gray scale background in Fig. 2(a) is segmented into only few clusters identifying the foreground character. In Fig. 2(b) we illustrate that for practical purposes, in this case detection of the license plate, even an intermediate iteration step, here $k=12$, may be used without need to wait for equilibration (at $k \approx 30$). Figure 2(c) shows the quality of segmentation for a highly complicated picture.

Data clustering becomes tremendously complicated when the intrinsic correlation between the data points which belong to the same cluster is small. A situation like this always occurs if the clusters extend into a thin, threadlike shape or an almost fractal structure, for example, when dealing with images of biomolecules, polymers, or stellar structures. The ECU makes better use of the energy landscape which underlies the clustering problem by *sharing energy* between the bond-freezing and the spin-update steps of the algorithm. The additionally introduced global inhibition enhances contrast. As a consequence the quality of the results improves and, most notably, energy sharing leads to an acceleration of the segmentation by about a factor of 10 [Fig. 1(h)].

In the course of development of the modern cluster update algorithms similar ideas have been proposed on sometimes more general grounds. Kandel and Domany [8] lay out how to preserve detailed balance for a broad class of algorithms and they show how several other proposed update variants [4] may be rephrased to comply with this. The ECU algorithm is also embedded in this framework. Niedermayer [7] shows that in the clustering step (1a) any function $p_{ij}^{(1)}(E_{ij})$ can be used in principle, but proposes for practical purposes to apply $p_{ij}^{(1)}=1-\exp[-\beta(E_{ij}-E_0)]$ with some appropriately chosen E_0. With this choice the contribution of the nonfrozen bonds to the update is clipped at E_0. In our case we share the energies in a proportional way between the clustering and update steps. The alignment of clusters is thus enhanced by also including the stronger bonds with higher energy content.

In summary, the recognition task of segmenting an image may be performed with high efficiency by a simple cluster update algorithm if global inhibition is implemented. Furthermore, we believe that our cluster update approach may also be useful for the simulation of other spin models as its efficiency is not dependent on the special properties of the Potts model we use here.

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