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LOOKING THROUGH WAVELETS TO VIEW THE ISING PROBLEM

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ABSTRACT

While there exist many coarse-graining techniques for accelerating Molecular Dynamic and Monte Carlo simulations, the rich structure and scaling properties of wavelets have found limited use in these techniques, especially in their investigating of thermodynamic properties of materials. To promote exploration in this field of molecular modeling, we apply wavelets to the solution of the simplest of models, the Ising model and evaluate the most fundamental of objects in statistical mechanics, the partition function, now based on a wavelet-modifed Hamiltonian. We extend [1] to use the Haar and db2 wavelets, as also wavelet packets to coarsely grain the 2-D finite size Ising model. Thermodynamic properties are then calculated to predict, in some sense, potential for phase transition. Exact calculations are confirmed using Monte Carlo simulations. Based on these results we propose a number of wavelet-based problems for further investigation.

Index Terms— Coarse Graining, Wavelets, Critical Exponents, Phase Transition, Multiscale Modeling.

1. INTRODUCTION

1.1. Motivation - The Ising Problem

One of the basic problems in statistical mechanics is to understand how short-range interactions such as interactions between molecules in a crystal affect long range correlative behavior [2]. A simple way to model these systems is through the Ising model: A lattice with N points (or molecules) are considered as N independent (state) variables. These variables, constrained to have binary values (such as up-down, occupied or unoccupied, or in general order-disorder) and *small scale* nearest-neighbor interactions, are subject to a change in parameter such as temperature or pressure. The concern is with the causal large-scale behavior of the state of the system. That is, determining critical points by measuring exponents in power laws - the *critical exponents*. Or equivalently, the singularity of the function. An example of such behavior is phase transition: Familiar illustrations are the change of water to ice, water to steam, solid-liquid-gas transitions, or more generally the non-analytical behavior of a thermodynamic quantity.

1.2. The Potts Model

The generalization of the Ising (2-state) model is the q-state Potts model. These two models are archetypes of systems with nearest-neighbor interactions. The Ising model has for example been used to study the microstructure evolution of grain boundaries and hence used to simulate the behavior of a bicrystal [3]. The Potts model has found use in many applications such as liquid-gas transitions, foam behavior, magnetism, biological membranes, spin glasses and tumor migration [4].

1.3. Renormalization Group & Wavelets

Like wavelets, the renormalization group (RG) transformation may be considered a coarse graining technique. Physically, in the context of the Ising model, RG recursively reduces spatial dimensionality by absorbing sites to create block variables. Up to this point, this is similar to retaining scaling coefficients in a wavelet transform. However, the recursive procedure in the RG transformation, in the limit to ∞, leads to convergence to so-called fixed points. When phase change does occurs, as in the 2-D Ising case, one of the several fixed points will correspond to the point (temperature for example) where phase transition occurs. That is, on either side of the point, the system "moves" away from that point. This is the point of non-analyticity - the singular point. Critical exponents α in $|T - T_c|^{-\alpha}$ where T, T_c are temperature and critical temperature respectively, and the partition function in the region $|T - T_c|$ can also be determined with the recursive procedure. A formal introduction to RG may be found in various texts, as for example [5], [6].

Coarse graining with wavelets, in a practical sense leads to a different interpretation. While progressive decomposition leads to coarser scales and dimensionality reduction, there is always the option, not possible in the RG, of retaining detail information. Indeed using wavelet packets as also maximum modulus coefficients allows both dimensionality reduction and invertibility. The latter is not possible with the RG.

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A vast selection of orthogonal and biorthogonal wavelets are available with the latter allowing storage of more energy in the low frequency subbands than the former. Consequently, a variety of interesting coarse grained models become available (with different computational costs), raising the possibility of new insight into the phase transition process. Finally, wavelets allow determination of Lipschitz exponents of singularities using wavelet modulus maxima. This could be applicable to the determination of critical exponents of thermodynamic functions exhibiting phase transitions at critical temperatures.

The Haar wavelet has been applied in coarse graining the Ising problem [1]. As in that work, we incorporate the identity operator $\mathbf{I} = \mathbf{W^T W}$ ($\mathbf{W}$ is the unitary Discrete Wavelet Transform (DWT) matrix) in the Hamiltonian. We extend that work with the Haar wavelet, to include, db2, and (Haar-based) wavelet packets in coarse graining the 2-D finite size Ising model. The partition function is calculated to establish exact values of magnetism. Monte Carlo simulations, with samples selected to reduce bias are employed to verify results. Only some of these simulations are presently shown in Section 3.

2. WAVELET-MODIFIED HAMILTONIAN

We consider the phase transition problem in ferromagnetism. This is formulated as an Ising problem on a size-N square lattice; that is, a lattice with N variables. We follow the conventional method of analysis. The Hamiltonian for the size-N, 2-dimensional Ising system with nearest-neighbor interaction is given by,

$$-\beta H = \sum_i h_i \sigma_i + \sum_i \sum_j J_{i,j} \sigma_i \sigma_j = \mathbf{h}^T \mathbf{u} + \mathbf{u}^T \mathbf{J} \mathbf{u} \quad (1)$$

where h_i is the strength of the external field at lattice site i, lattice variable $\sigma_i = \pm 1$, $J_{i,j}$ is the strength of the interactions between sights i and j, and $\beta = (k_B T)^{-1}$. State vector $\mathbf{u} = [\sigma_1, \sigma_2, \ldots, \sigma_N]^T$ and $\mathbf{J}$ is the $N \times N$ connectivity matrix.

2.1. Orthogonal Wavelet Transform

A coarse representation of the lattice variables is best achieved through application of a unitary transform. The usual filter bank design assumes an infinite-length signal. Since both the variables $\mathbf{u}$ and connectivity matrix $\mathbf{J}$ are finite, this results in a distortion at the boundaries. The usual way around this difficulty is to assume the finite signal as a segment of an infinite one formed by a periodic replication of the finite signal. Since discontinuities created at the boundary can lead to artifacts, periodic symmetric extensions are often considered. This leads to linear phase filters and bi-orthogonal filter banks constrained by symmetric filter requirements.

Following [1], an orthogonal discrete wavelet transform $\mathbf{W}$ is applied to the 1-D vector of variables $\mathbf{u}$ and to the 2-D coupling strengths $\mathbf{J}$. The wavelet transform $\mathbf{W}$ will not be limited to the Haar wavelet as assumed in (ibid.). For the finite size N lattice, the $N \times N$ orthogonal wavelet transform $\mathbf{W}$ is introduced in equation (1) as $\mathbf{W^T W} = \mathbf{I}$ to give,

$$-\beta H = \mathbf{h}^T \mathbf{W^T W u} + \mathbf{u}^T \mathbf{W^T W J W^T W u} \quad (2)$$

Hence we have,

$$-\beta H = \tilde{\mathbf{h}}^T \tilde{\mathbf{u}} + \tilde{\mathbf{u}}^T \tilde{\mathbf{J}} \tilde{\mathbf{u}} \quad (3)$$

where $\tilde{\mathbf{h}} = \mathbf{Wh}$, $\tilde{\mathbf{u}} = \mathbf{Wu}$ and $\tilde{\mathbf{J}} = \mathbf{WJW^T}$.

Note that $\tilde{\mathbf{u}}$ and $\tilde{\mathbf{J}}$ may contain more spin directions and long-range interactions respectively than before. For the one-level wavelet decomposition the Hamiltonian is written as,

$$-\beta H = \tilde{\mathbf{h_1}}^T \tilde{\mathbf{u_1}} + \tilde{\mathbf{h_2}}^T \tilde{\mathbf{u_2}} + \tilde{\mathbf{u_1}}^T \tilde{\mathbf{J}}_{\mathbf{1},1} \tilde{\mathbf{u_1}} +$$

$$\tilde{\mathbf{u_1}}^T \tilde{\mathbf{J}}_{1,\mathbf{2}} \tilde{\mathbf{u_2}} + \tilde{\mathbf{u_2}}^T \tilde{\mathbf{J}}_{\mathbf{2},1} \tilde{\mathbf{u_1}} + \tilde{\mathbf{u_2}}^T \tilde{\mathbf{J}}_{\mathbf{2},2} \tilde{\mathbf{u_2}} \quad (4)$$

Retaining any of the scales reduces dimensionality. The reduced dimension low pass $\tilde{\mathbf{u_1}}^T \tilde{\mathbf{J}}_{\mathbf{1},\mathbf{1}} \tilde{\mathbf{u_1}}$ may be decomposed for a second-level decomposition generating yet more coarse grain sub-Hamiltonians. The corresponding partition function $Z = \sum_i e^{-\beta H(u_i)}$, probabilities $P(u_i) = \frac{e^{-\beta H(u_i)}}{Z}$, magnetism $M(u_i) = \frac{1}{N} \sum_{i=1}^{N \times N} s_i$ and expected magnetism $<M> = \sum_{i=1}^{N \times N} P(u_i) M(u_i)$ are calculated for all states u_i, for any Hamiltonian or sub-Hamiltonian. Each of the latter provide a coarse-grain realization.

3. SIMULATIONS

We consider the Ising problem on a 16×16 lattice with no external field and follow the decomposition described in Section 2.1. Figure 1 shows the original coupling strengths $\mathbf{J}$ (1) of the non-transformed lattice. Coupling strengths $\tilde{\mathbf{J_1}}, \tilde{\mathbf{J_2}}, \tilde{\mathbf{J_3}}$ represent three levels of wavelet decomposition of $\mathbf{J}$ using the 2-D Haar wavelet transform (2), (3) applied three times. At each application, only the low pass energies (top left regions 8×8, 4×4 and 2×2 in $\tilde{\mathbf{J_1}}, \tilde{\mathbf{J_2}}, \tilde{\mathbf{J_3}}$ respectively) and corresponding reduced dimension vectors $\mathbf{u}$ of size 8×1, 4×1 and 2×1 are preserved. These give the three coarse grain model descriptions. Magnetism with respect to temperature, for the original and the three coarse-grained macroscopic structures are shown in Figure 2. Figure 3 shows the low pass energies utilized for each of the 4 cases. Note that since energy is preserved in orthogonal transforms the decrease in energy is that due to the remaining high pass coefficients that are not utilized.

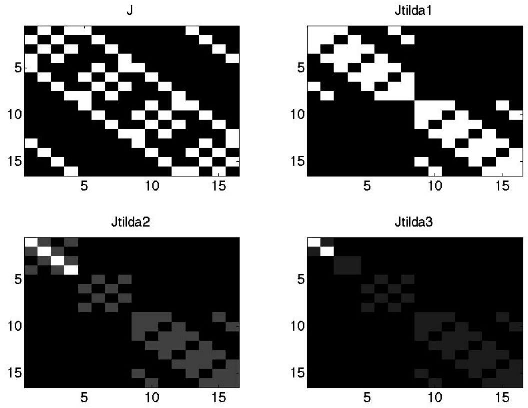

Fig. 1. Interaction Strengths $J, \tilde{J}_1, \tilde{J}_2, \tilde{J}_3$

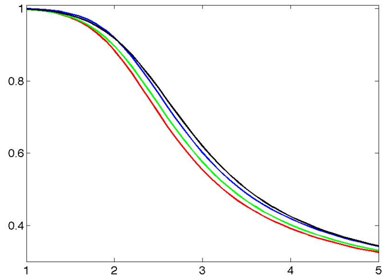

Fig. 2. Magnetism with Coarse Graining

4. Research Problems

There are an abundance of problems, of a rich variety, that can be considered in the use of wavelets for investigating a fundamental problem, phase transition, in statistical mechanics. The probability of finding a particular mesoscopic configuration in the Ising model is expressed in terms of the probability function of the partition function, which is expressed in terms of the wavelet-modified Hamiltonian as described in Section 2.1

Practical problems in the investigation of the wavelet-based Hamiltonian would include the following: (i) evaluating the role of detail coefficients in the evolution of phase transitions; (ii) determination of best biorthogonal wavelet basis for concentrating energy in low frequency subbands; (iii) coarse graining using wavelet packets as also using wavelet maximum modulus coefficients to allow both invertibility and reconstruction; (iv) estimating computation cost and error in the proposed coarse graining techniques; (v)using wavelet maximum modulus coefficients to estimate singularities with Lipschitz constants; (vi) application to Monte Carlo and Molecular Dynamic simulations.

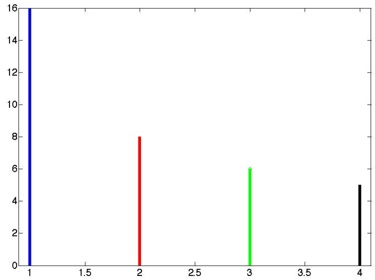

Fig. 3. Energies with Coarse Graining

Perhaps the most intriguing, difficult and potentially promising problem would be the understanding the relationship between RG transformations and continuous wavelets, and the application of the latter to identifying phase transition. As noted earlier, one of the limitations of the RG method is its inherent inability to perfectly reconstruct after coarse graining, a shortcoming that wavelets can avoid at the expense of retaining all detail coefficients. The panoply of wavelet bases and efficient wavelet transforms offers enticing new possibilities for finding optimal theoretical and computational compromises between these competing dynamics, particular in multi-dimensional systems where the Ising model has only been effectively investigated by Monte Carlo methods. Additional theoretical insight might also be garnered by seeking to relate the action of the Renormalization (semi-)Group on certain (Sobolev) spaces of functions to affine group actions on these spaces, as alluded to in [7]. Such connections may further illuminate the relation between the RG and wavelet approaches.

4. CONCLUSION

We have used wavelets in the solution of the 2-D finite size Ising model as an example to illustrate some of the general ideas about phase transition. Small scale systems where exact enumeration is possible have been used. While explicit occurrence of non-analytic behavior is not possible for such systems, the potential for phase transition has been observed. Various wavelet-based ideas are proposed for further investigation.

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