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2-DIMENSIONAL FRUSTRATION MODELING

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2-Dimensional Frustration Modeling

Synopsis:

Computational frustration modeling can be used to study systems such as spin glasses and cuprate vortex states. Frustration is due to competing and random interactions. Our general model can be mapped into a harmonic-oscillator model or an Ising model. Monte Carlo simulations are used to study frustration relaxation in a 2-dimensional lattice.

2-Dimensional Frustration Modeling

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Abstract. Frustration is due to competing and random interactions among spins, atoms, or in general, characters. Computational methods can be used to study frustrated systems such as spin glasses, cuprate vortex states, and also social behaviors. We define a general frustrated model in which frustration of each character is proportional to the square of the relative distance between the actual and ideal (or assigned) positions. This model can be mapped into harmonic oscillators or an Ising model. We record the total frustration as a function of time for characters' motion, to see how they minimize their frustration in a two-dimensional lattice and reach their lowest frustration. We utilize Monte Carlo simulations to study at absolute zero the frustration relaxation for different number of characters, and for different assigned distances. Characters assigned to regular structures such as Thomson Figures show exponential relaxation. For a character set, where the ideal assignments are a row (or a column) we observe unusual behaviour. At early times, the frustration relaxes to zero; yet after reaching zero, the frustration jumps up to non-zero values; later, the frustration becomes exactly zero and the row is formed.

1 Introduction

One of the recent, important concepts in condensed matter is frustration. Spin glasses, cuprate vortex states and any kind of glassy material are some of the physical systems in which frustration exists. One also observes this phenomenon in biophysical processes such as protein folding [1]. Computational methods are a good way to study frustration in a two-dimensional system. [2] We study the behavior of frustration for a set of characters on a square lattice at zero temperature. We set characters such that they start to move from random positions, then record the behavior of characters in their pursuit of minimizing their frustration [3].

2 Frustration modeling

2.1 Two-Dimensional Model [2-4]

We define frustration F_i for each character i on a square lattice as

$$F_i = \sum_{i \neq j} (D_{ij} - I_{ij})^n, \quad (1)$$

where n can be an integer number, D_{ij} is the actual distance between characters i and j, and I_{ij} is the assigned distance. I_{ij} is not necessarily equal to I_{ji} while $D_{ij} = D_{ji}$. I_{ij} can be chosen to be equal (E) $I_{ij} = E$ for all $i \neq j$ and $I_{ii} = 0$, or they can be chosen to be random, or the row/column (RC), $I_{ij} = |i - j|$ creating rows or columns. We define I'_{ij}, where $I'_{ij} = I_{ij} \; \forall \; i \neq j$ and $I_{ii} = 0$. $I'_{ij} = E$ creates Thomson-like figures. The total frustration $\mathrm{F_{tot}}$ is the sum over individual frustrations F_i:

$$F_{tot} = \sum_i F_i \ . \qquad (2)$$

For n=2 in eqn (1) F_{tot} is similar to a harmonic potential for which characters build a virtual network that are connected by springs [5]. The characters' potential is different only by their spring constant (k). Applying this similarity, the potential energy of the network is given by:

$$U_{tot} = \sum_i U_i, \qquad (3)$$

$$U_i = \sum_{\substack{j \\ i\neq j}} \frac{k_{ij}}{2}\left(r_{ij} - r_{ij}^0\right)^2, \qquad (4)$$

where r_{ij} and r_{ij}^0 are the instantaneous and equilibrium distances between characters i and j, respectively, $r_{ij} = \sqrt{\frac{2}{k_{ij}}}\, D_{ij}$ and $r_{ij}^0 = \sqrt{\frac{2}{k_{ij}}}\, I_{ij}$.

Our frustration model can also be mapped to an Ising model [6]. We expand eqn (2) as follows:

$$F_{tot} = \sum_{i\neq j}(D_{ij} - I_{ij})^2 = \sum D_{ij}\left(D_{ij} - 2I_{ij}\right) + \sum I_{ij}^2 = -\sum d_{ij}^+ d_{ij}^- + const, (5)$$

where $d_{ij}^\pm = I_{ij} \pm d_{ij}$, $d_{ij} = I_{ij} - D_{ij}$ and $const = \sum I_{ij}^2$. This expression is similar to an Ising Hamiltonian.

2.2 Method

Our aim is to find how frustration relaxes towards an F_{tot} minimum. Minimization of F_{tot} can be interpreted as finding the correct arrangement of characters with respect to other characters and the assigned, imposed "order" I_{ij}, or of "disorder" from the prearranged "ideal" setting.

We start the simulation with random or specific positions of characters at time zero. Each character (i) is allowed to minimize its own frustration by moving one step in a direction of its lowest F_i. If the frustration of a character cannot be minimized, the character does not move. We use a Monte Carlo algorithm allowing all characters to move one step; thus causing the total frustration to decrease in the beginning. Yet in the long run, we see different time-dependent F_{tot} behaviors, depending on I_{ij}. This algorithm is "capitalistic" in nature, as each character lowers only its own frustration. That does not automatically mean F_{tot} gets lowered.

Our algorithm is discussed in more detail below. At time zero, we choose random positions for all characters and based on eqn (1) we calculate the frustration of each characters (F_{iold}).

For the next time step, we move every character in the two-dimensional lattice.

Our algorithm has the following rules:

0. Sort characters based on order of frustration (F_i) from the highest F_i to the lowest and set i=1.
1. Take a character i with F_{iold}=F_i.
2. Find the new position of character i. This new position is one of its neighbors.
3. Check if this new position is occupied. If occupied, go back to rule 2.
4. If its eight neighbors are occupied go to rule 9.
5. Find the lowest frustration among the unoccupied neighbors of character i and call it F_{inew}.
6. Calculate for character i: $\Delta_i = \delta(F_{inew} - F_{iold})$ where δ is a T-related coefficient.
7. If $\Delta_i \leq 0$, move the character i to the new position and go to rule 9.
8. If $\Delta_i > 0$, move the character i to the new position by probability P:
   a. If temperature is zero (T=0): P=0.

b. If the temperature is nonzero: $P=\exp(-\Delta_i/k_BT)$. Then generate random number R, $0 \le R \le 1$.
c. If $P \ge R$, move the character i to the new position and go to rule 9.
d. If $P < R$, move back to the old position of character i and go to rule 9.

9. i=i+1 and go back to rule 1.

Repeat rules 1-9 for all characters. Then go to the next time step and iterate rules 0-9 to obtain the total frustration (F_{tot}), using eqn (2).

3 Relaxation behavior of frustration for different number of characters and different I'_{ij}

We present the results of our T = 0 simulations, with three, four, and five characters with two different types of I'_{ij}: E and RC. Characters are on a two-dimensional square lattice (20×20). In these cases, we first investigate the time dependence of frustration (F_{tot}) and then compare fitting the relaxation of frustration to linear, power and exponential functions, $F_{tot}(t) = \alpha + \beta t$, $F_{tot}(t) = \alpha t^{-\beta}$ and $F_{tot}(t) = \alpha\exp(-\beta t)$, to find the best fit to determine the nature of the frustration relaxation.

3.1 *The $I'_{ij} = 4$ case: Five characters*

We start with $I'_{ij} = \begin{pmatrix} 0 & 4 & 4 & 4 \\ 4 & 0 & 4 & 4 \\ 4 & 4 & 0 & 4 \\ 4 & 4 & 4 & 0 \end{pmatrix}$ at zero temperature. As shown in Fig 1, F_{tot} relaxes exponentially with $\mathrm{FRUS}(t) = 1.43\times10^3\exp(-0.347t)$. The minimum frustration figure is a pentagon-like shape on the square lattice.

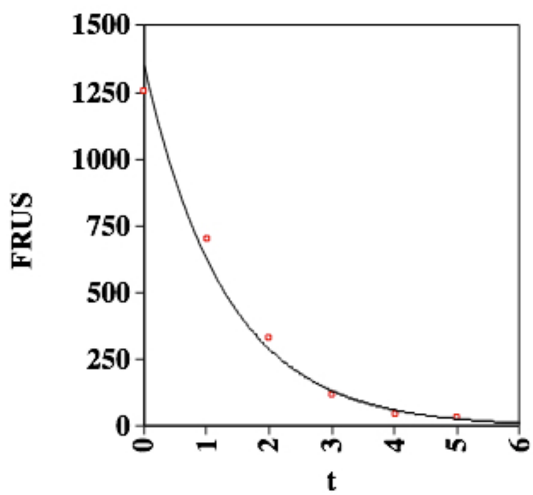

Figure 1. For five characters in a 20×20 lattice when $I'_{ij} = 4$, frustration relaxes to 18.9 at t=6 with exponential behavior, $FRUS(t) = 1.43\times10^3\exp(-0.347t)$.

3.2 The $I'_{ij} = 5$ case

3.2.1 Three characters

We put three characters randomly on a 20×20 lattice. With $I'_{ij} = \begin{pmatrix} 0 & 5 & 5 \\ 5 & 0 & 5 \\ 5 & 5 & 0 \end{pmatrix}$ 20 time steps are performed at T = 0. In Fig 2, F_{tot} is plotted as a function of time and the frustration relaxes with an exponential behavior: FRUS(t)=6.82×10^2exp(-0.556t). The final position of characters forms a triangle on the lattice.

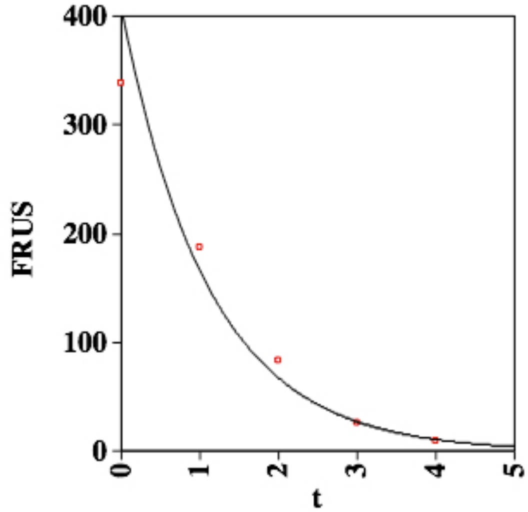

Figure 2. Three characters on a 20×20 lattice where I'_{ij} = 5. Frustration relaxes to 0.32 and the best fit is an exponential with FRUS(t)=6.82×10^2exp(-0.556t).

3.2.2 *Four characters*

We set the dimensions of the lattice to 20×20 and put four characters randomly on the lattice. Select $I'_{ij} = 5$ and F_{tot} relaxes exponentially: $\mathrm{FRUS(t)} = 1.04\times10^3\exp(-0.263\mathrm{t})$ as shown in Fig 3. The final character positions make a trapezium.

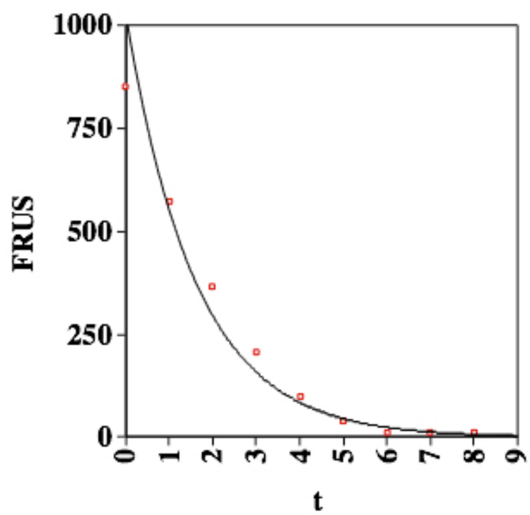

Figure 3. Four characters on a 20×20 lattice with $I'_{ij} = 5$. Frustration relaxes to 8.59 at t=9. The best fit is $\mathrm{FRUS(t)} = 1.04\times10^3\exp(-0.263\mathrm{t})$.

3.2.3 *Five characters*

We take $I'_{ij} = 5$. We again get a pentagon-like shape similar to $I'_{ij} = 4$. Frustration relaxes exponentially with $\mathrm{FRUS(t)} = 1.13\times10^3\exp(-0.288\mathrm{t})$. See Fig 4.

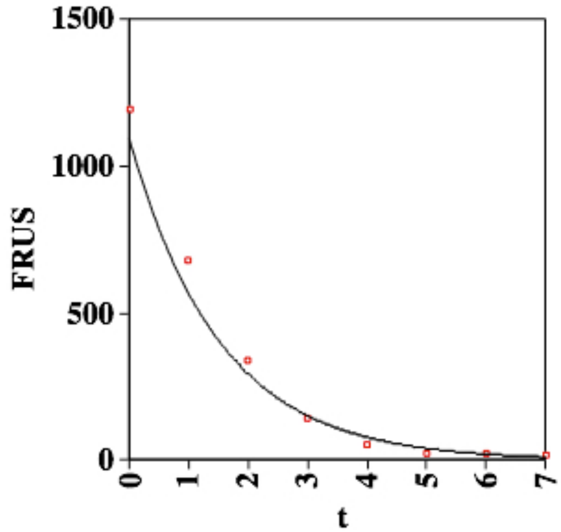

Figure 4. Five characters on a 20×20 lattice and $I'_{ij} = 5$. FRUS(t) relaxes to 28.6 at t=7 exponentially and the best fit is $\mathrm{FRUS(t)} = 1.13\times10^{3}\exp(-0.288\mathrm{t})$.

3.3 The row/column case

3.3.1 The row3/column case

We take $I_{ij} = |i-j| = \begin{pmatrix} 0 & 1 & 2 \\ 1 & 0 & 1 \\ 2 & 1 & 0 \end{pmatrix}$. Frustration relaxes to zero and the characters align in a row on the lattice. In Fig 5 the frustration relaxes to $\mathrm{FRUS(t)} = 6.54\times10^{2}\exp(-0.432\mathrm{t})$. In the initial stage, the frustration relaxes to its lowest value, close to zero. While frustration goes to zero, there are small fluctuations, around the minimum frustration for $5 < t < 9$, the magnitude of the fluctuations is about 10. However in the later stage ($t \geq 9$), the frustration relaxes exactly to zero with exponential behavior and the row is formed. We discuss these fluctuations in section 3.4

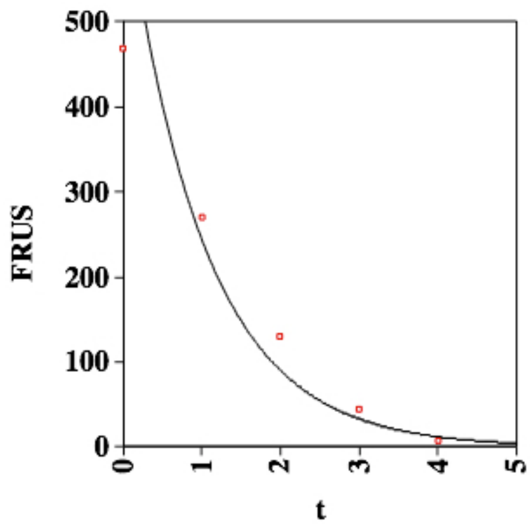

Figure 5. FRUS relaxes to zero on a 20×20 lattice for three characters and $I_{ij} = |i-j|$. The best fit is $\mathrm{FRUS(t)} = 6.54\times10^{2}\exp(-0.432t)$.

3.3.2 The row4/column case

We take $I_{ij} = |i-j| = \begin{pmatrix} 0 & 1 & 2 & 3 \\ 1 & 0 & 1 & 2 \\ 2 & 1 & 0 & 1 \\ 3 & 2 & 1 & 0 \end{pmatrix}$. Frustration relaxes to zero and the characters align in a row on the lattice. In Fig 6 the frustration relaxes to $\mathrm{FRUS(t)} = 2.07\times10^3\exp(-0.265\mathrm{t})$. Similar to three characters, the frustration relaxes to its lowest value at t=6, close to zero. While the frustration goes to zero, there are fluctuations around the minimum frustration for $6 < t < 9$, its magnitude of fluctuations is about 20. However in the later stage, the frustration relaxes exactly to zero with exponential behavior and the row is formed.

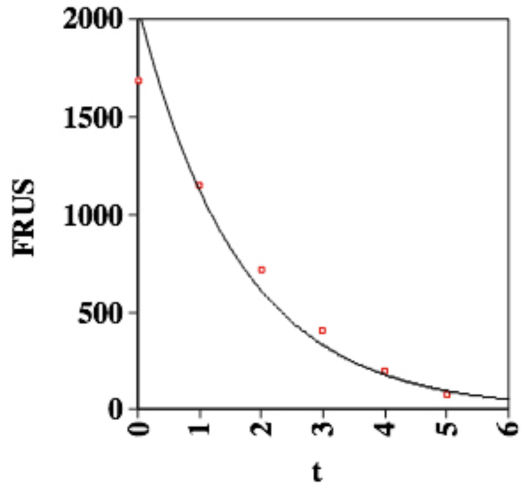

Figure 6. FRUS relaxes to zero on a 20×20 lattice for four characters when $\mathrm{I_{ij}} = |\mathrm{i}-\mathrm{j}|$. The best fit is $\mathrm{FRUS(t)} = 2.07\times10^3\exp(-0.265\mathrm{t})$.

3.3.3 The row5/column case

We take $I_{ij} = |i-j| = \begin{pmatrix} 0 & 1 & 2 & 3 & 4 \\ 1 & 0 & 1 & 2 & 3 \\ 2 & 1 & 0 & 1 & 2 \\ 3 & 2 & 1 & 0 & 1 \\ 4 & 3 & 2 & 1 & 0 \end{pmatrix}$. Frustration relaxes to zero and all characters align in a row on the lattice. An exponential fit yields $\mathrm{FRUS(t)} = 4.2\times10^3\exp(-0.30\mathrm{t})$ with a regression coefficient $r^2 = 0.9$. The low r^2 indicates, the fit is not good. Plotting Log(FRUS) as a function of time (Fig 7), we observe two linear behaviors, which suggests two processes are in play for the time intervals: $0 \leq t \leq 4$ and $5 \leq t \leq 8$. The best fits for these two regimes are $\mathrm{Log(FRUS(t))} = -0.21\mathrm{t} + 3.5$ and $\mathrm{Log(FRUS(t))} = -0.49\mathrm{t} + 4.6$ resp. Hence, the frustration initially relaxes and then transitions to a faster relaxation process.

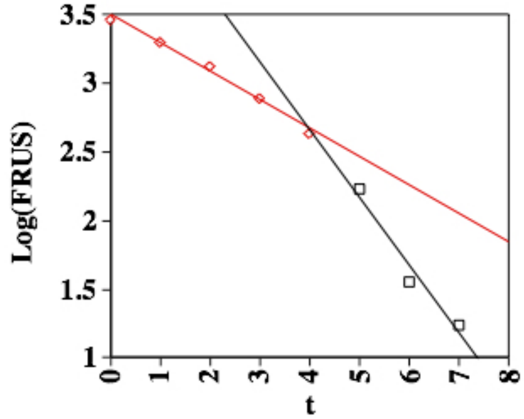

Figure 7. Log(FRUS) shows two regimes with each regime shows a different linear behavior for a 20×20 lattice and five characters when $I_{ij} = |i - j|$. The best fit is $\mathrm{Log(FRUS(t))} = -0.21t + 3.5$ for $0 \leq t \leq 4$ (red line) and $\mathrm{Log(FRUS(t))} = -0.49t + 4.6$ for $5 \leq t \leq 7$ (black line).

3.4 Row/Column Frustration behavior

For the row/column cases, we have observed unusual F_{tot} relaxation. There are fluctuations in an intermediate time period. These behaviors are observed for three, four and five characters as mentioned in sections 3.3.1, 3.3.2 and 3.3.3. Hence indicating, this type of fluctuations is independent of the number of characters. In Fig 8, these fluctuations are plotted for the 5-characters case. The frustration initially relaxes close to its lowest value. Then F_{tot} reaches close to zero at t=9, followed by fluctuations around the minimum frustration between t=9 to 17. The magnitude of the fluctuations is about 60 in this time interval and then the frustration relaxes exactly to zero at t=18 when the row is formed. By comparing frustration of three, four and five characters, we see the time of fluctuations as well as the interval that characters are fluctuating increases by increasing the number of characters. Its minimum frustration is found and finally a row is formed. The source of those fluctuations could be related to local minima, close to zero frustration.

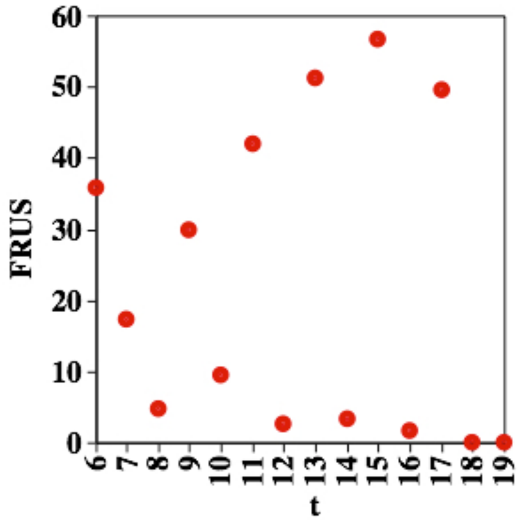

Figure 8. Frustration for five characters, $I_{ij} = |i - j|$ in the time interval [6, 19]. The frustration relaxes close to its minimum value at t=8. Between t=9 to 17 there are fluctuations. After t=17, the frustration relaxes exactly to zero and the characters form a row.

4 Summary

For two E and RC sets, we have calculated the total frustration as a function of time for characters' motion to see how they relax and minimize their frustration on a two-dimensional 20×20 lattice. In table I results are summarized together with the regression coefficient r^2.

Table I. Frustration results are for a 20×20 lattice at zero temperature. The results are fitted with three functions, as discussed in section 3. r^2 is the regression coefficient with $r^2 = 1$ indicating a perfect fit. Characters assigned to regular figures show exponential behavior. For a character set, where the ideal assignments are, a row (or column) we also observe exponential relaxation.

Characters	I_{ij}	r^2 Linear	r^2 Power	r^2 Exponential
3	5	0.85	0.75	**0.93**
4	5	0.95	0.87	**0.97**
5	5	0.77	0.96	**0.98**
5	4	0.84	0.93	**0.99**
3	RC	0.93	0.86	**0.95**
4	RC	0.94	0.87	**0.97**

How the characters move to reach the lowest frustration is investigated for two cases $I'_{ij} = E$ and $I_{ij} = |i - j|$ for 3, 4 and 5 characters. We utilize Monte Carlo simulations to study the frustration relaxation for different number of characters and for different assigned distances. Characters assigned to regular structures such as Thomson Figures show exponential behavior. For a character set, where the ideal assignments are a row (or column) we observe unusual behavior. In the initial stage, the frustration relaxes to its lowest value, which is close to zero. However, we observe fluctuations around the minimum frustration; in the later stage, the frustration relaxes exactly to zero with an exponential behavior and the row is formed. We also observed that for a five characters set, where the ideal assignments are a row (or column), there are two regions of relaxations. At initial times, the system relaxes and then switches to a faster relaxation for larger times.

Acknowledgments

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