Project Weak-Schur: Ising Model Proposal

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1 Hamiltonian Function 1

We are searching for a colouring of the first N natural numbers into n colours, such that whenever $\exists(a, b, c) \in [N]$ and $a + b = c$, then a, b and c do not share the same colour. The following have been modelled after the decision variables and functions presented in [1], Section 6.

Definition 1. *The decision variable $x_{m,c}$ is defined as*

$$x_{m,c} := \begin{cases} 1 & Col(m) = c \\ 0 & else \end{cases} \tag{1}$$

This defines the matrix of decision variables $\boldsymbol{x} \in M_{N\times n}(\{0, 1\})$.

Definition 2. *The Hamiltonian function for a Schur partition of the first N natural numbers into n colors is the following.*

$$\mathcal{H}_S(\boldsymbol{x}) := A\sum_{i=1}^{N}\left(1 - \sum_{c=1}^{n} x_{i,c}\right)^2 + B\sum_{i,j=1}^{N}\sum_{c=1}^{n} x_{i,c}x_{j,c}x_{i+j,c} \tag{2}$$

where $A, B \in \mathbb{R}_{\geq 0}$ are arbitrary weights.

We now add a constraint to define the Hamiltonian for the Weak Schur case.

Definition 3. *The Hamiltonian function for a Weak Schur partition of the first N natural numbers is the following.*

$$\mathcal{H}_{WS}(\boldsymbol{x}) \tag{3}$$

$$:= \underbrace{A\sum_{i=1}^{N}\left(1 - \sum_{c=1}^{n} x_{i,c}\right)^2}_{\mathcal{A}} + \underbrace{B\sum_{i,j=1}^{N}\sum_{c=1}^{n} x_{i,c}x_{j,c}x_{i+j,c} \cdot (2N - |i - j|)}_{\mathcal{B}} \tag{4}$$

where $A, B \in \mathbb{R}_{\geq 0}$ are arbitrary weights.

1.1 Remarks on Definitions

We make some remarks on the first sum $\mathcal{A}$ first.

1. $\mathcal{A}$ penalises the assignment of multiple colors to a single number.

Now, we study $\mathcal{B}$.

1. Notice that for any good triplet, (i, j, k), $l_{i,j} = x_{i,c}x_{j,c}x_{i+j,c} = 0$, we have $x_{i,c} = 0$, or $x_{i+j,c} = 0$, without loss of generality, which immediately implies that they do not share the colour c.
2. Suppose that they all share the same colour, then, $l_{i,j} = 1$, and the energy penalty becomes positive in $\mathcal{B}$.
3. In the degenerate case when $i = j$, $|i - j| = 0$, and $\mathcal{B}$ is effectively maximised by a multiplication with $2N$, even if it satisfies the sum-free constraints. This implies only weakly sum-free triplets can attain a minimal $\mathcal{B}$. Intuitively, $\mathcal{B}$ is minimised whenever i and j are "far apart".

1.2 Problem Visualisation

The problem is essentially an n-dimensional Ising problem with N charges.

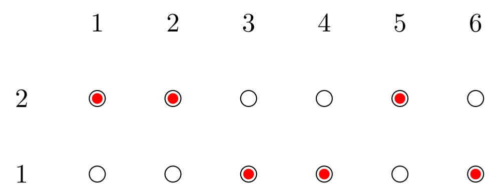

Figure 1: Ising Model Representation of the partition $\{\{1,2,5\},\{3,4,6\}\}$ into n=2 colours. Here, Red = +1, White = -1.

1.3 Computational Aspects

To simplify the computation of the Hamiltonian, we can use the following looping order:

$$\mathcal{B}_{WS}(\boldsymbol{x}) = B\sum_{c=1}^{n}\sum_{i=1}^{N} x_{i,c}\sum_{j=1}^{N} x_{j,c}x_{i+j,c}(2N-|i-j|)$$

A simple Simulated Annealing algorithm can be proposed to find minimal configurations[1] for a given N, n, similarly to a simulated annealing approach, as follows in Alg. 1. Other approaches can be implemented from [2], [3], [4] and [5].

Algorithm 1: Simulated Annealing solution

Data: $T_{max}, T_{min} \geq 0$, $N, n \in \mathbb{N}$
Result: $x \in M_{N\times n}(\{-1,1\})$
$x \overset{\$}{\leftarrow} M_{N\times n}(\{-1,1\})$;
$T \leftarrow T_{max}$;
while $T > T_{min}$ **do**
  $r, c \overset{\$}{\leftarrow} [1:N]\times[1:n]$;
  $x^{\text{new}}_{r,c} \leftarrow -x_{r,c}$;
  if $\mathcal{H}_{WS}(x^{new}) \leq \mathcal{H}_{WS}(x)$ **then**
    $x \leftarrow x^{\text{new}}$;
  else
    if $e^{-\frac{\mathcal{H}_{WS}(x^{new})-\mathcal{H}_{WS}(x)}{T}} < \alpha$ **then**
      $x \leftarrow x^{\text{new}}$;
    end
  end
end

1.4 Optimisation Formulation

Alternatively, we can formulate the problem as a constrained, non-linear, integer optimisation problem in the following way.

$$\min_{\boldsymbol{x}\in\{1,-1\}^N} H_{WS}(\boldsymbol{x}) \tag{5}$$

[1] Usually local minima

Using the constraints, we get that

$$\min_{\boldsymbol{x}\in\{1,-1\}^N} \mathcal{B}(\boldsymbol{x})$$
$$\text{subject to: } \forall c,\ \langle \mathbb{1}, x_{\cdot,c}\rangle = 1$$

or, considering $\boldsymbol{x} \in M_{N\times n}(\{1,-1\})$,

$$\min_{\boldsymbol{x}\in\{1,-1\}^N} \mathcal{B}(\boldsymbol{x}) \tag{6}$$
$$\text{subject to: } \langle \mathbb{1}, \boldsymbol{x}\rangle = \mathbb{1} \tag{7}$$

1.5 Decoding

Here, the decoding is straightforward: A valid decoding can only be performed when the partition satisfies all the constraints i.e. if $\mathcal{H} = 0$, then reading each row of the matrix $[x_{i,c}]_{N\times n}$ gives us the right colour for each number. Else, $[x_{i,c}]_{N\times n}$ will give potential partitions, for each resolution, each with some energy, and we can take the minimal configuration.

2 Hamiltonian Function 2

Alternatively, we can choose a different decision variable, where each variable can be thought of as a certificate.

Definition 4. *The decision variable $x_{m,k}$ is defined as*

$$x_{m,n} := \begin{cases} 1 & Col(m) = Col(n) \\ 0 & else \end{cases} \tag{8}$$

So, $x_{i,j} = x_{j,i} = 1 \implies i$ and j have the same colour. Note that this does not impose any constraint on the number of colours necessary; only that in the most general sense, for a desired partition of N numbers, $x_{i,j}$ have the same colour, or not.

Therefore, we can simplify the corresponding Hamiltonians as follows.

Definition 5. *The Hamiltonian function for a Schur partition of the first N natural numbers is the following.*

$$\mathcal{H}^C := A\sum_{i,j=1}^{N} x_{i,j}x_{i,i+j}x_{j,i+j}$$

Definition 6. *The Hamiltonian function for a Weak Schur partition of the first N natural numbers is the following.*

$$\mathcal{H}^C_{WS} := A\sum_{i,j=1}^{N} x_{i,j}x_{i,i+j}x_{j,i+j}\cdot|i-j|$$

In a similar manner to Eqn. 3, the $|i-j|$ multiplier penalises the degenerate case of $2i = k$, where the only possible way to decrease $\mathcal{H}_{WS}^{C}$ is to maintain distinct colors for $x_{i,j}$, $x_{i,i+j}$ and $x_{j,i+j}$.

2.1 Decoding

Since the Hamiltonian does not impose the colour-constraint, the Decoding algorithm must. The proposal is a type of Branching algorithm, that has the signature: **Decode**: $([x_{i,j}]_{N\times N}, n) \to C \in [N] \times [n]$, where $[N] = \{1, 2, \ldots, N\}$ and n is the number of colours.

Informally, the steps are as follows:

1. **Initialisation** Assign a random colour to the first number $k = 1$.
2. For each number $k > 1$, for each certificate $x_{k,m} = 1$ where $m \neq k$,
   (a) if m has a colour, assign k the same colour and terminate.
3. If not terminated yet, for all certificates $x_{k,m} = 0$ $(m \neq k)$, create a list $L = [1 : n]$
   (a) for each $x_{k,m} = 0$, remove m from L.
   (b) Branch on the size of L:
      i. if $|L| = 0$, terminate with error.
      ii. If $|L| = 1$ i.e. $L = \{m\}$, assign k the colour m and terminate.
      iii. Else, branch on all possible values that remain in L.

References

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