MPF objective function for an Ising model

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This document derives the MPF objective function for the case of an Ising model. In Section 1, connectivity is set between all states which differ by a single bit flip. In Section 2, an additional connection is included between states which differ in all bits. This additional connection is particularly beneficial in cases (such as spike train data) where unit activity is extremely sparse.

The MPF objective function is

$$K\left(\mathbf{J}\right) = \sum_{\mathbf{x}\in\mathcal{D}} \sum_{\mathbf{x}'\notin\mathcal{D}} g\left(\mathbf{x},\mathbf{x}'\right) \exp\left(\frac{1}{2}\left[E(\mathbf{x};\mathbf{J}) - E(\mathbf{x}';\mathbf{J})\right]\right), \tag{1}$$

where $g\left(\mathbf{x},\mathbf{x}'\right) = g\left(\mathbf{x}',\mathbf{x}\right) \in \{0,1\}$ is the connectivity function, $E(\mathbf{x};\mathbf{J})$ is an energy function parameterized by $\mathbf{J}$, and $\mathcal{D}$ is the list of data states. For the Ising model, the energy function is

$$E\left(\mathbf{x};\mathbf{J}\right) = \mathbf{x}^T\mathbf{J}\mathbf{x} \tag{2}$$

where $\mathbf{x} \in \{0,1\}^N$, $\mathbf{J} \in \mathcal{R}^{N\times N}$, and $\mathbf{J}$ is symmetric ($\mathbf{J} = \mathbf{J}^T$).

1 Single bit flips

We consider the case where the connectivity function $g\left(\mathbf{x},\mathbf{x}'\right)$ is set to connect all states which differ by a single bit flip,

$$g\left(\mathbf{x},\mathbf{x}'\right) = \left\{ \begin{array}{ccc} 1 & \mathbf{x} \text{ and } \mathbf{x}' \text{ differ by a single bit flip,} & \sum_n |x_n - x'_n| = 1 \\ 0 & \text{otherwise} & \end{array}\right. . \tag{3}$$

The MPF objective function in this case is

$$K\left(\mathbf{J}\right) = \sum_{\mathbf{x}\in\mathcal{D}} \sum_{n=1}^{N} \exp\left(\frac{1}{2}\left[E(\mathbf{x};\mathbf{J}) - E(\mathbf{x}+\mathbf{d}(\mathbf{x},n);\mathbf{J})\right]\right) \tag{4}$$

where the sum over n is a sum over all data dimensions, and the bit flipping function $\mathbf{d}(\mathbf{x},n) \in \{-1,0,1\}^N$ is

$$\mathbf{d}(\mathbf{x},n)_i = \left\{ \begin{array}{cc} 0 & i \neq n \\ -(2x_i - 1) & i = n \end{array}\right. \tag{5}$$

For the Ising model, this MPF objective function becomes (using the fact that $\mathbf{J} = \mathbf{J}^T$)

$$K(\mathbf{J}) = \sum_{\mathbf{x}\in\mathcal{D}} \sum_n \exp\left(\frac{1}{2}\left[\mathbf{x}^T\mathbf{J}\mathbf{x} - (\mathbf{x} + \mathbf{d}(\mathbf{x},n))^T\mathbf{J}(\mathbf{x} + \mathbf{d}(\mathbf{x},n))\right]\right) \tag{6}$$

$$= \sum_{\mathbf{x}\in\mathcal{D}} \sum_n \exp\left(\frac{1}{2}\left[\mathbf{x}^T\mathbf{J}\mathbf{x} - \left(\mathbf{x}^T\mathbf{J}\mathbf{x} + 2\mathbf{x}^T\mathbf{J}\mathbf{d}(\mathbf{x},n) + \mathbf{d}(\mathbf{x},n)^T\mathbf{J}\mathbf{d}(\mathbf{x},n)\right)\right]\right) \tag{7}$$

$$= \sum_{\mathbf{x}\in\mathcal{D}} \sum_n \exp\left(-\frac{1}{2}\left[2\mathbf{x}^T\mathbf{J}\mathbf{d}(\mathbf{x},n) + \mathbf{d}(\mathbf{x},n)^T\mathbf{J}\mathbf{d}(\mathbf{x},n)\right]\right) \tag{8}$$

$$= \sum_{\mathbf{x}\in\mathcal{D}} \sum_n \exp\left(-\frac{1}{2}\left[2\sum_i x_i J_{in}\left(1 - 2x_n\right) + J_{nn}\right]\right) \tag{9}$$

$$= \sum_{\mathbf{x}\in\mathcal{D}} \sum_n \exp\left(\left[\left(2x_n - 1\right)\sum_i x_i J_{in} - \frac{1}{2}J_{nn}\right]\right). \tag{10}$$

Assume the symmetry constraint on $\mathbf{J}$ is enforced by writing it in terms of another possibly asymmetric matrix $\mathbf{J}' \in \mathcal{R}^{N\times N}$,

$$\mathbf{J} = \frac{1}{2}\mathbf{J}' + \frac{1}{2}\mathbf{J}'^T. \tag{11}$$

The derivative of the MPF objective function with respect to $\mathbf{J}'$ is

$$\begin{aligned}\frac{\partial K\left(\mathbf{J}'\right)}{\partial J'_{lm}} = {} & \frac{1}{2}\sum_{\mathbf{x}\in\mathcal{D}} \exp\left(\left[\left(2x_m - 1\right)\sum_i x_i J_{im} - \frac{1}{2}J_{mm}\right]\right)\left[\left(2x_m - 1\right)x_l - \delta_{lm}\frac{1}{2}\right] \\ & + \frac{1}{2}\sum_{\mathbf{x}\in\mathcal{D}} \exp\left(\left[\left(2x_l - 1\right)\sum_i x_i J_{il} - \frac{1}{2}J_{ll}\right]\right)\left[\left(2x_l - 1\right)x_m - \delta_{ml}\frac{1}{2}\right],\end{aligned} \tag{12}$$

where the second term is simply the first term with indices l and m reversed.

Note that both the objective function and gradient can be calculated using matrix operations (no for loops). See the code.

2 All bits flipped

We consider the case where the connectivity function $g\left(\mathbf{x}, \mathbf{x}'\right)$ is set to connect all states which differ by a single bit flip, and all states which differ in all bits,

$$g\left(\mathbf{x}, \mathbf{x}'\right) = \begin{cases} 1 & \mathbf{x} \text{ and } \mathbf{x}' \text{ differ by a single bit flip,} \quad \sum_n \left|x_n - x'_n\right| = 1 \\ 1 & \mathbf{x} \text{ and } \mathbf{x}' \text{ differ in all bits,} \quad \sum_n \left|x_n - x'_n\right| = N \\ 0 & \text{otherwise} \end{cases}. \tag{13}$$

This extension to the connectivity function aids MPF in assigning the correct relative probabilities between data states and states on the opposite side of the state space from the data, even in cases (such as sparsely active units) where the data lies only in a very small region of the state space.

The modified objective function has the form,

$$K\left(\mathbf{J}\right) = K_{single}\left(\mathbf{J}\right) + K_{all}\left(\mathbf{J}\right). \tag{14}$$

We can take the first term, which deals only with single bit flips, from Equation 10,

$$K_{single}\left(\mathbf{J}\right) = \sum_{\mathbf{x}\in\mathcal{D}}\sum_{n}\exp\left(\left[\left(2x_n - 1\right)\sum_i x_i J_{in} - \frac{1}{2}J_{nn}\right]\right). \tag{15}$$

The second term is

$$\begin{aligned} K_{all} &= \sum_{\mathbf{x}\in\mathcal{D}}\exp\left(\frac{1}{2}\left[E(\mathbf{x};\mathbf{J}) - E(\mathbf{1}-\mathbf{x};\mathbf{J})\right]\right) && (16)\\ &= \sum_{\mathbf{x}\in\mathcal{D}}\exp\left(\frac{1}{2}\left[\mathbf{x}^T\mathbf{J}\mathbf{x} - \left(\mathbf{1}-\mathbf{x}\right)^T\mathbf{J}\left(\mathbf{1}-\mathbf{x}\right)\right]\right), && (17)\end{aligned}$$

where $\mathbf{1}$ is the vector of all ones.

The contribution to the derivative from the second term is

$$\frac{\partial K_{all}}{\partial J_{lm}} = \frac{1}{2}\sum_{\mathbf{x}\in\mathcal{D}}\exp\left(\frac{1}{2}\left[\mathbf{x}^T\mathbf{J}\mathbf{x} - \left(\mathbf{1}-\mathbf{x}\right)^T\mathbf{J}\left(\mathbf{1}-\mathbf{x}\right)\right]\right)\left[x_l x_m - \left(1-x_l\right)\left(1-x_m\right)\right]. \tag{18}$$