Inferring the Underlying Structure of Spin Glass Model

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Introduction

The Ising Model arises from the field of Statistical Mechanics. It has been applied to study gene regulatory networks by representing genes as binary variables (on/off states) and modeling the interactions between them. A spin glass model consists of N binary spins s_i, $i = 1, 2, ..., N$ with $s_i = \pm 1$, These spins are coupled by a coupling matrix J_{ij} and are subject to an external magnetic field H_i, which is the bias term in our application. The energy of such configuration is given by the Hamiltonian:

$$H(\vec{s}) = -\sum_{i,j} s_i J_{ij} s_j - \sum_i H_i s_i$$

The configuration probability is given by $\frac{e^{-\beta H}}{Z}$ where $\beta > 0$ is the inverse temperature and Z is the normalising constant.

Spin Glass Model Inference

Given sample of size N, $\vec{s}^{\mu}$, $\mu = 1, 2, ..., N$ from a spin glass model with unknown parameters, to compute the coupling matrix and the bias term, we use the maximum likelihood approach:

$$\begin{aligned} L(\vec{J}, \vec{H}) &= \sum_{i,j} J_{ij} \frac{1}{N} \sum_{\mu} s_i^{\mu} s_j^{\mu} + \sum_i H_i \frac{1}{N} \sum_{\mu} s_i^{\mu} - \log Z(\vec{J}, \vec{H}) \\ &= \sum_{i,j} J_{ij} \langle \sigma_i \sigma_j \rangle^D + \sum_i H_i \langle \sigma_i \rangle^D - \log Z(\vec{J}, \vec{H}) \end{aligned}$$

Differentiated with respect to J and H we have:

$$\frac{\partial L}{\partial J_{ij}} = \langle \sigma_i \sigma_j \rangle^D - \langle \sigma_i \sigma_j \rangle \qquad \frac{\partial L}{\partial H_i} = \langle \sigma_i \rangle^D - \langle \sigma_i \rangle$$

The $\langle \sigma \rangle^D$ is the sample average and the $\langle \sigma \rangle$ is the expectation of the model fitted. At the maximum of the log-likelihood these derivatives are zeros. Two algorithms **Gradient Descent** and **Proximal Gradient Descent** are then applied to search for the optimal parameters

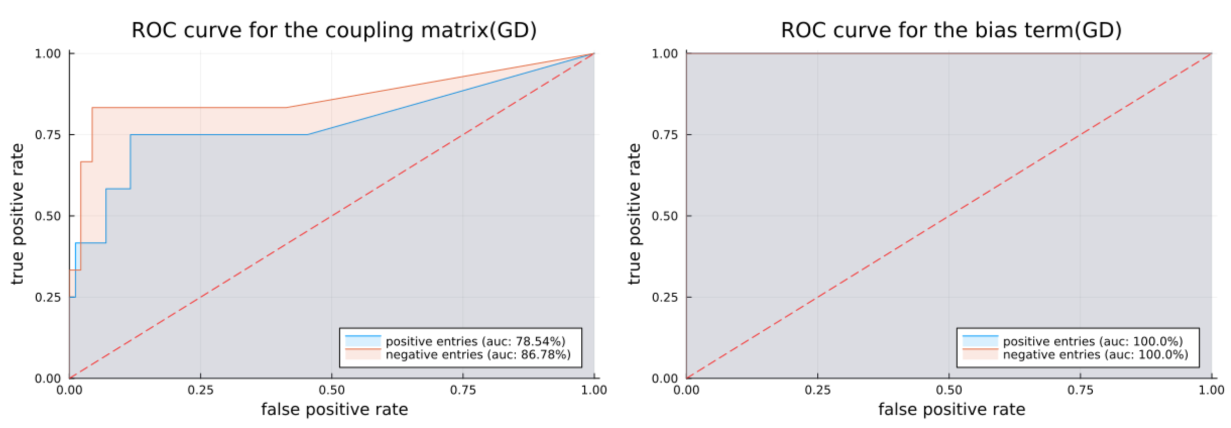
Gradient Descent(GD)

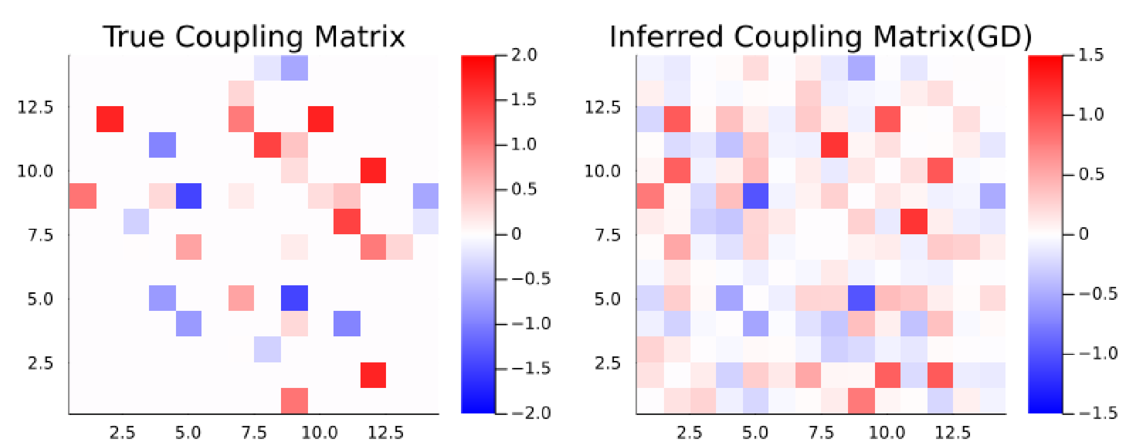
The log-likelihood is a concave function, therefore, we use a gradient descent approach. With learning rate λ, at each step, the coupling matrix and the bias are updated according to:

$$J_{ij}^{t+1} = J_{ij}^t + \lambda \frac{\partial L}{\partial J_{ij}}(\vec{J}^n, \vec{H}^n) \qquad H_i^{t+1} = H_i^t + \lambda \frac{\partial L}{\partial H_i}(\vec{J}^n, \vec{H}^n)$$

Given our focus on discerning positive and negative interactions among genes, our model's efficacy is assessed within a categorical spectrum.

The Area Under the Curve(AUC) of the Receiver Operating Characteristic(ROC) is used to evaluate model performance, with values between 1 and 0.5, where a larger AUC indicates better performance.





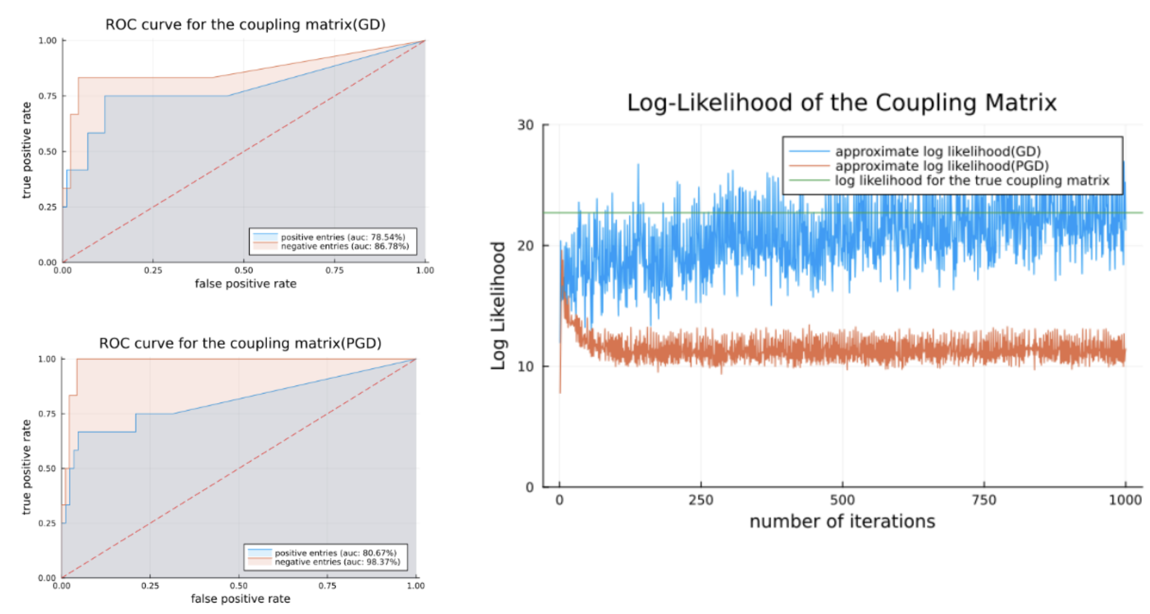
Proximal Gradient Descent(PGD)

Proximal Gradient Descent with Lasso Regularization promote sparsity in the inferred coupling matrix and improve model accuracy under the sparsity assumption.

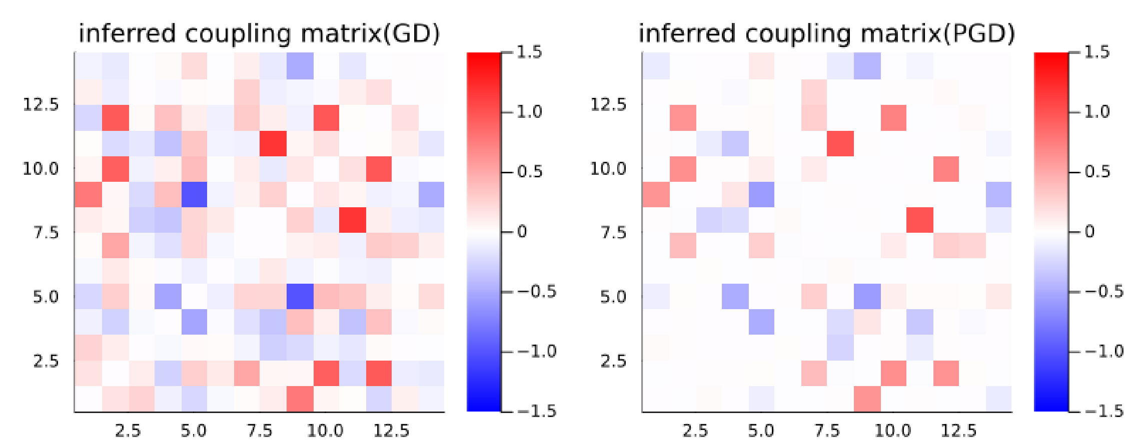
$$J_{ij}^{t+1} = \mathbf{prox}_{\beta_1 h}\left(J_{ij}^t + \lambda \frac{\partial L}{\partial J_{ij}}(\vec{J}^n, \vec{H}^n)\right) \qquad H_i^{t+1} = \mathbf{prox}_{\beta_2 h}\left(H_i^t + \lambda \frac{\partial L}{\partial H_i}(\vec{J}^n, \vec{H}^n)\right)$$

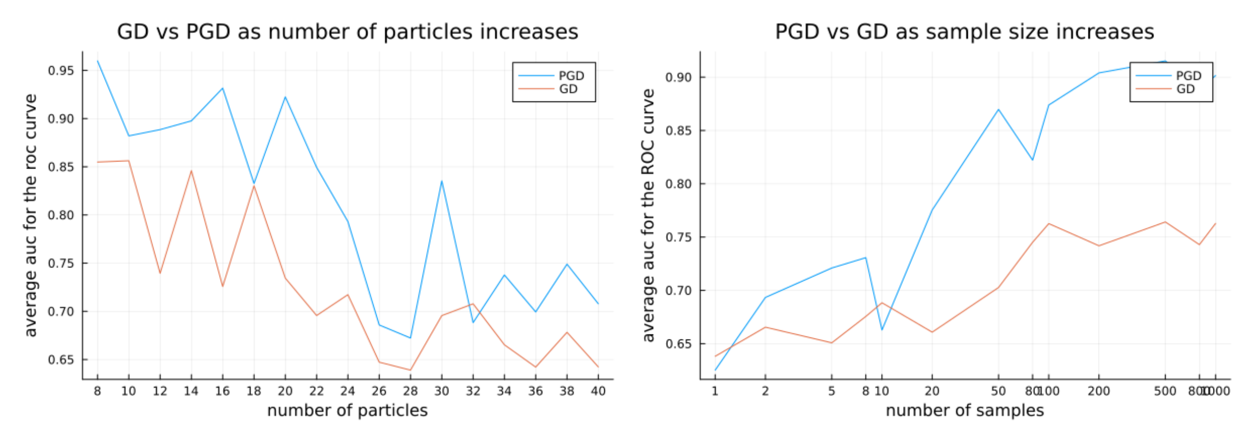
The proximal function is defined as

$$\mathbf{prox}_{\beta h}(u) = \begin{cases} u - \beta & u > \beta \\ 0 & -\beta < u \leq \beta \\ u + \beta & u < -\beta \end{cases}$$



PGD prevents the model from overfitting to the noise of the data and help recover the true underlying coupling between spins.





References

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