Project on Machine Learning

Alfred Alocias Mariadason

June 27, 2018

- Ising Model
- Metha et al, arXiv 1803.08823 accompanied by a Jupyter notebook.

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- Coupling constant

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- Coupling constant
- Phases
  - Ordered
  - Critical
  - Disordered

Linear Regression

- $\{y_i, \boldsymbol{x}_i\}_{i=1}^{n}$, $i = 1, \ldots, n$
- $\boldsymbol{y} = \boldsymbol{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}$
- minimize the L_2-norm $\min_{\boldsymbol{\beta}} \left| \boldsymbol{X}\boldsymbol{\beta} - \boldsymbol{y} \right|^2$
- Solution: $\boldsymbol{\beta}_{\mathrm{LS}} = \underset{\boldsymbol{\beta}}{\operatorname{argmin}} \left| \boldsymbol{X}\boldsymbol{\beta} - \boldsymbol{y} \right|^2 \Rightarrow \boldsymbol{\beta}_{\mathrm{LS}} = \left(\boldsymbol{X}^T \boldsymbol{X} \right)^{-1} \boldsymbol{X}^T \boldsymbol{y}$

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Ridge Regression

- L_2-regularization: $\boldsymbol{y} = \boldsymbol{X}\boldsymbol{\beta} + \alpha \sum_{i=1}^{m} \beta_i^2$
- $\boldsymbol{\beta}_{\text{Ridge}} = \operatorname{argmin}_{\boldsymbol{\beta}} \left(\left| \boldsymbol{X}\boldsymbol{\beta} - \boldsymbol{y} \right|^2 + \alpha \left| \boldsymbol{\beta} \right|^2 \right) \Rightarrow \boldsymbol{\beta}_{\text{Ridge}} = \left(\boldsymbol{X}^T \boldsymbol{X} + \alpha \boldsymbol{I} \right)^{-1} \boldsymbol{X}^T \boldsymbol{y}$

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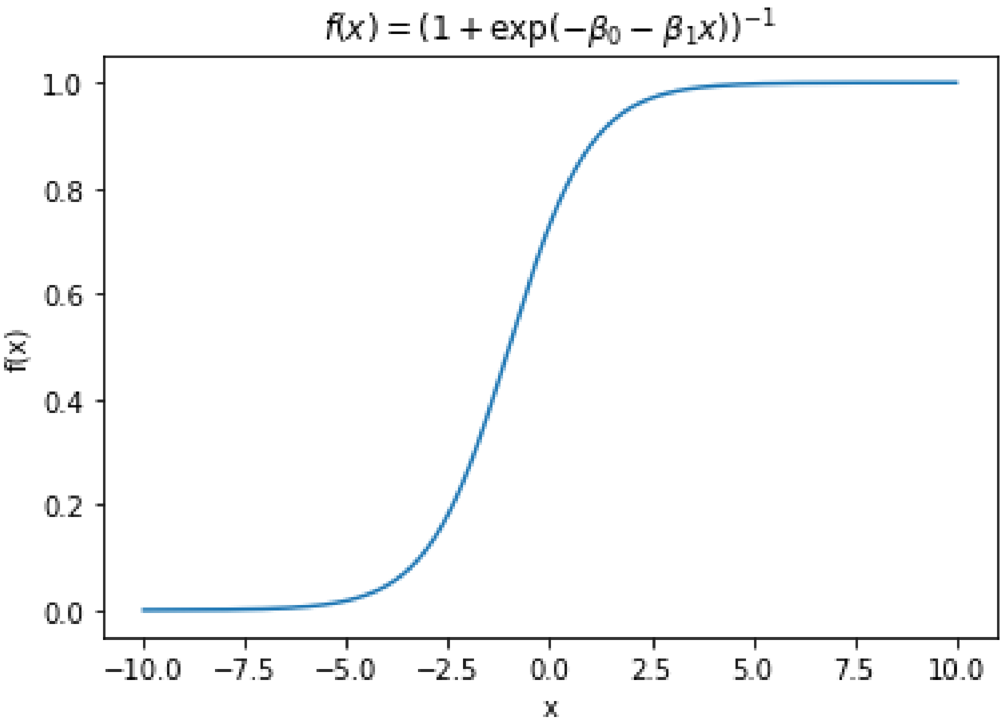
Lasso Regression

- L_1-regularization: $\boldsymbol{y} = \boldsymbol{X\beta} + \alpha \sum\limits_{i=1}^{m} \left|\beta_i\right|$
- Constrained ($|\boldsymbol{\beta}| \leq t$): $\boldsymbol{\beta}_{\mathrm{Lasso}} = \operatorname*{argmin}\limits_{\boldsymbol{\beta}} \left(\left|\boldsymbol{X\beta} - \boldsymbol{y}\right|^2 + \alpha\left|\boldsymbol{\beta}\right|\right)$
- Solution: $\beta_j^{\mathrm{Lasso}} = \operatorname{sign}\left(\beta_j^{\mathrm{LS}}\right)\left(\left|\beta_j^{\mathrm{LS}}\right| - \alpha\right)_+$

Logistic Regression

- Fit to sigmoid $f(x) = \frac{1}{1+\exp(-\boldsymbol{x}^T \boldsymbol{w})}$



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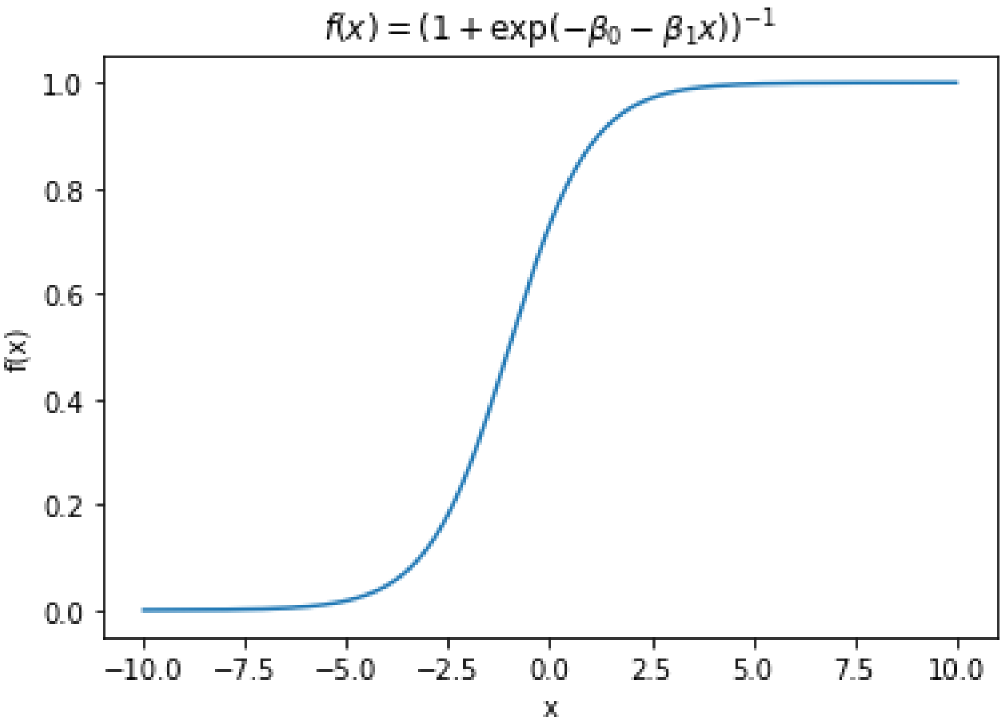

- Categorisation

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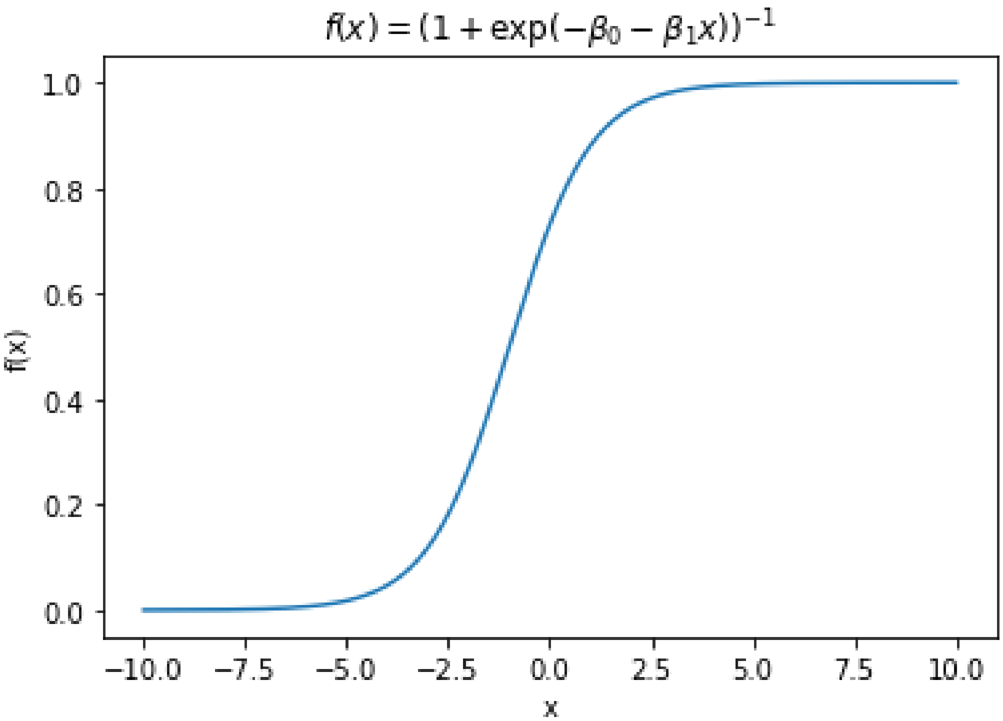

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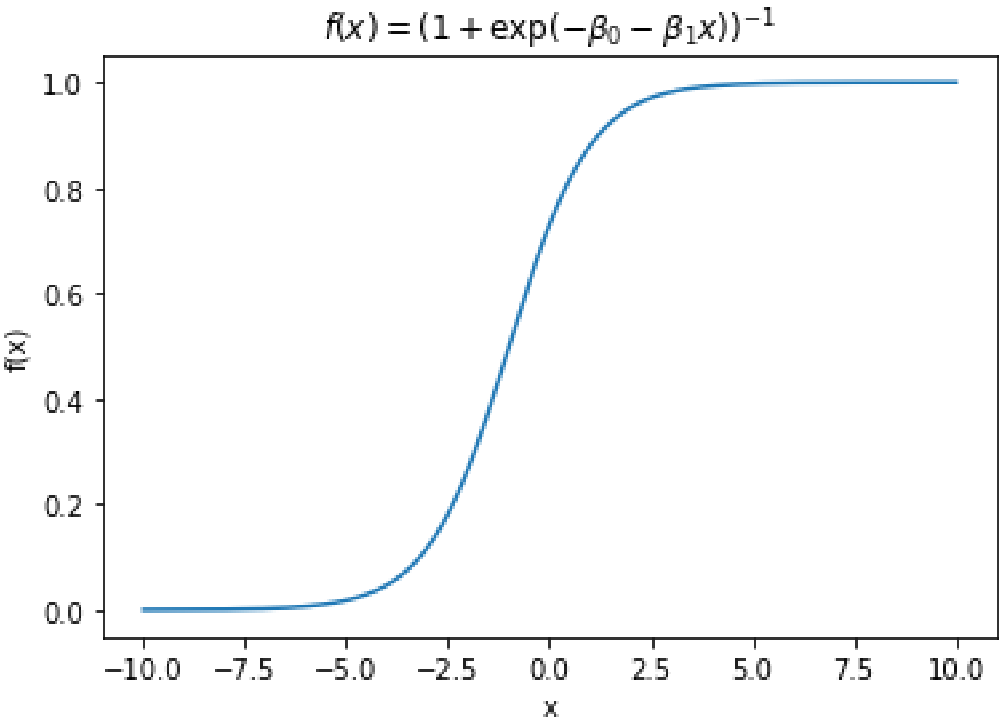

- Categorisation
  - Binary: $P(Y|X)$
- Cost: $C(\boldsymbol{w}) = -\sum_{i=1}^{n} \left[Y_i \log\left(f\left(\boldsymbol{X}_i^T\boldsymbol{w}\right)\right) + (1 - Y_i)\log\left(1 - f\left(\boldsymbol{X}_i^T\boldsymbol{w}\right)\right)\right]$

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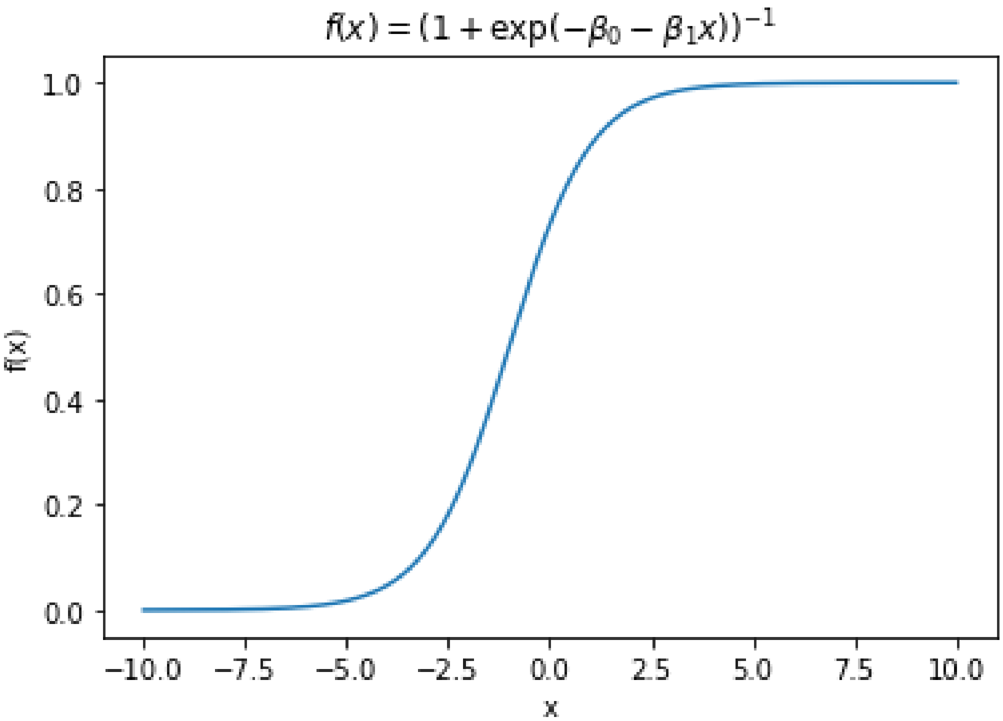

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- Numerical minimization: $\mathbf{0} = \nabla C(\boldsymbol{w}) = \sum_{i=1}^{n} \left[f \left(\boldsymbol{X}_i^T \boldsymbol{w} \right) - Y_i \right] \boldsymbol{X}_i$

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- Extremized Random Forest: Split decision trees at random

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- Backpropagation:
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  - **Feedforward**: Compute z^l and a^l for subsequent layers
  - **Error at output**: Calculate error in output
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- Cost function

Estimating the Coupling Constant of the 1D Ising Model

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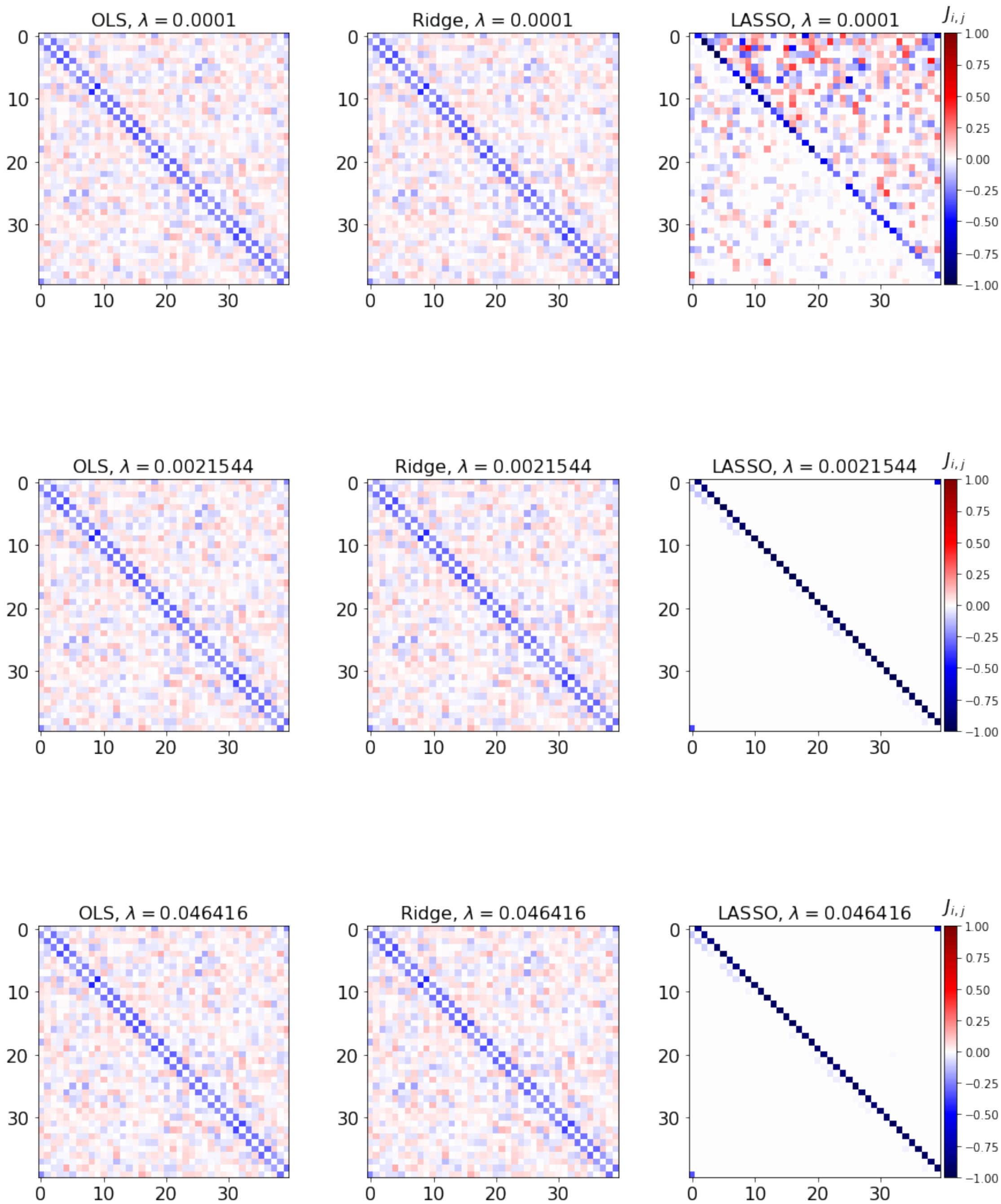
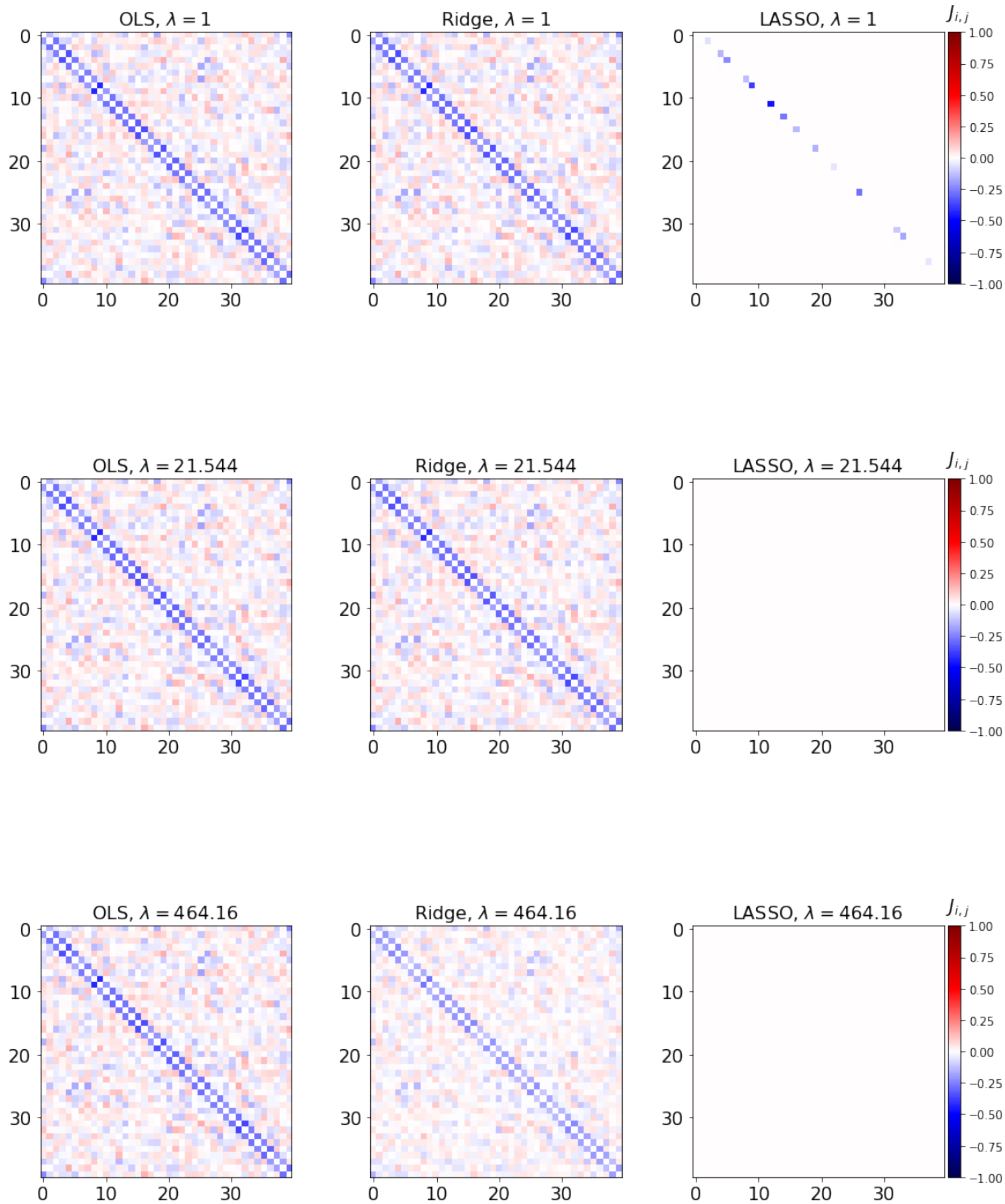
- $E^{(i)} = -\boldsymbol{X}^{(i)} \cdot \boldsymbol{J}$

Estimating the Coupling Constant of the 1D Ising Model



Estimating the Coupling Constant of the 1D Ising Model



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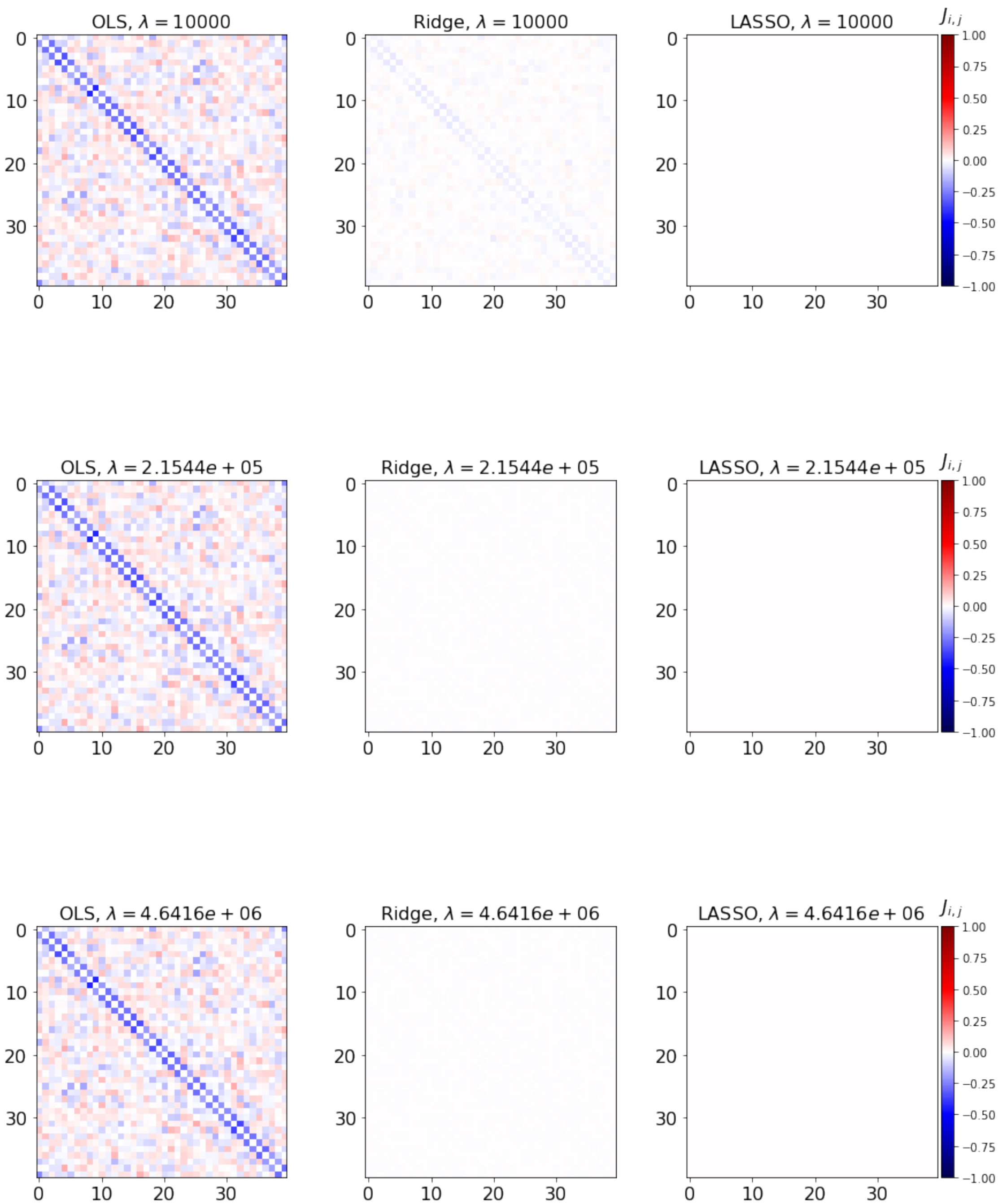

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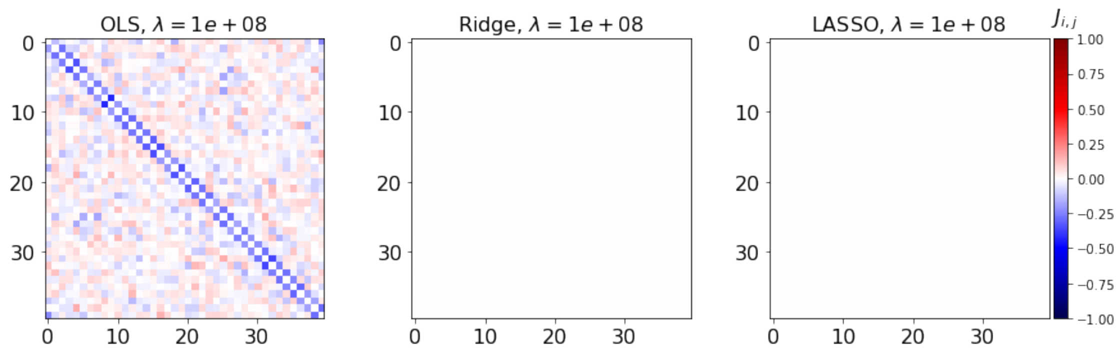

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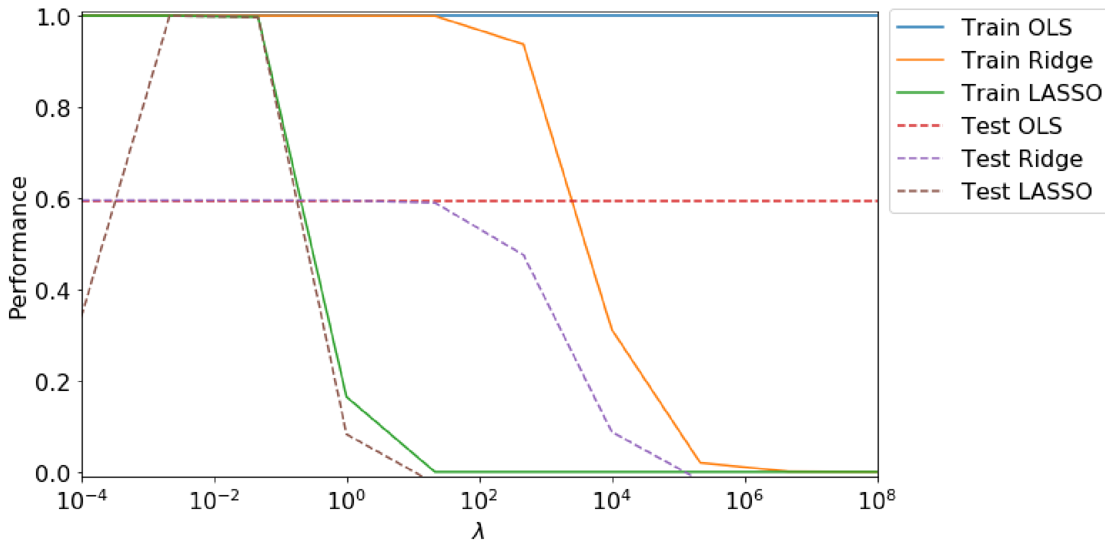
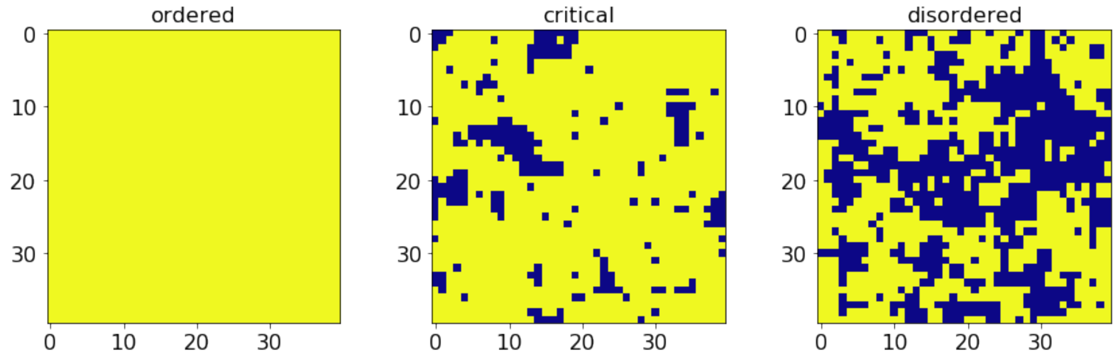


Determine the Phase of the Two-Dimensional Ising Model



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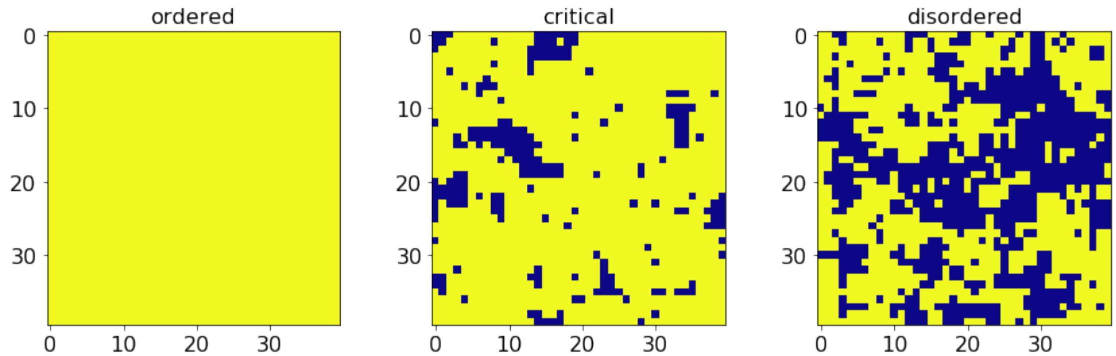

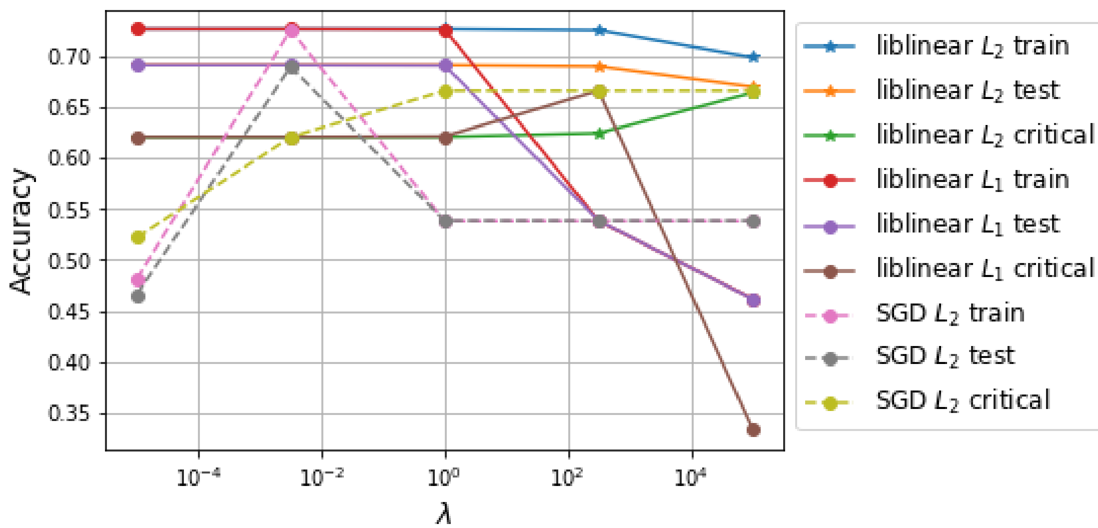

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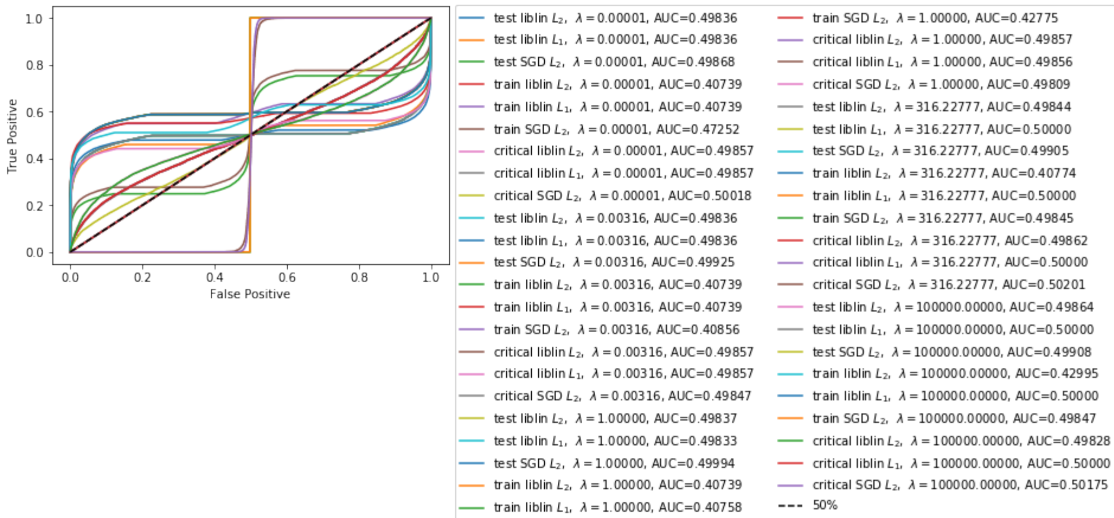
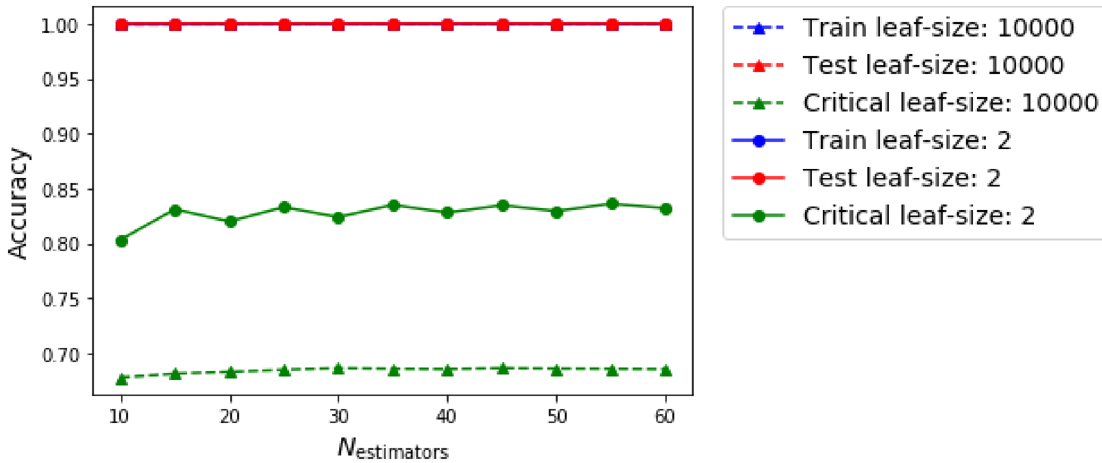


0.0.1 Using Random Forest to Classify Phases in the Ising Model



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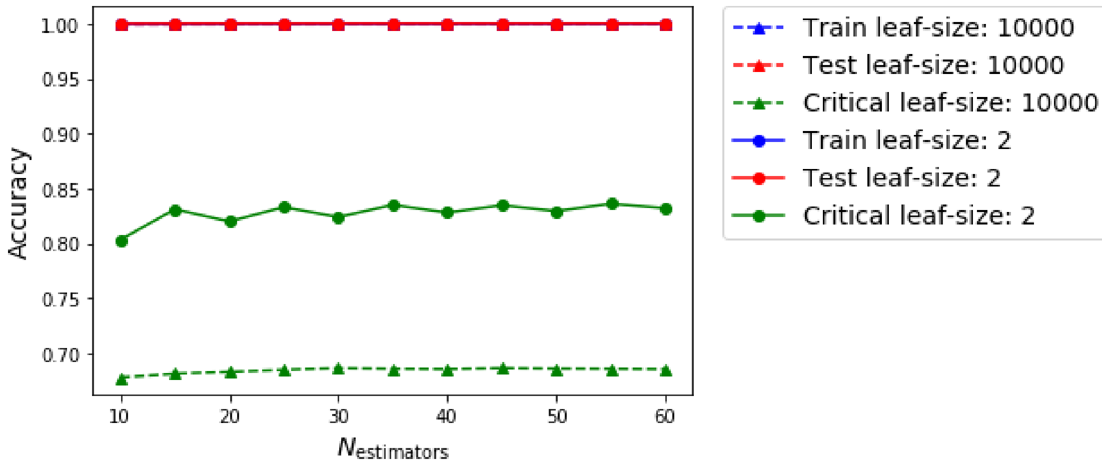

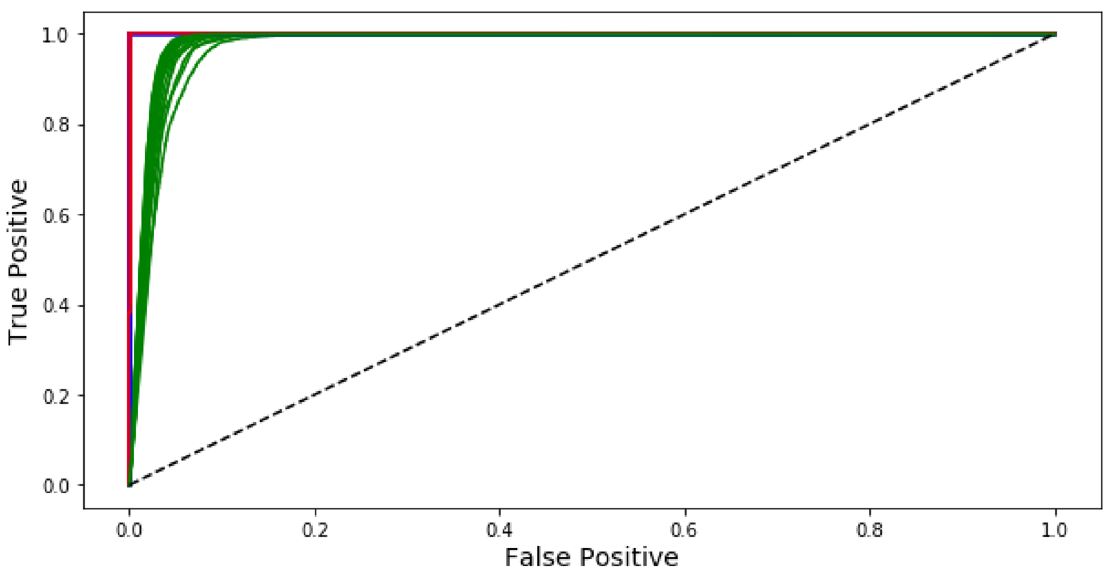

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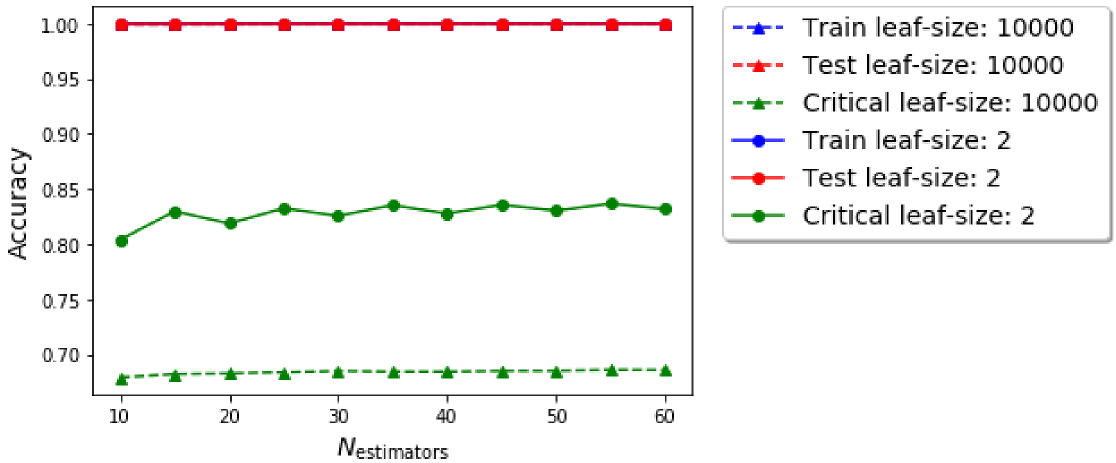

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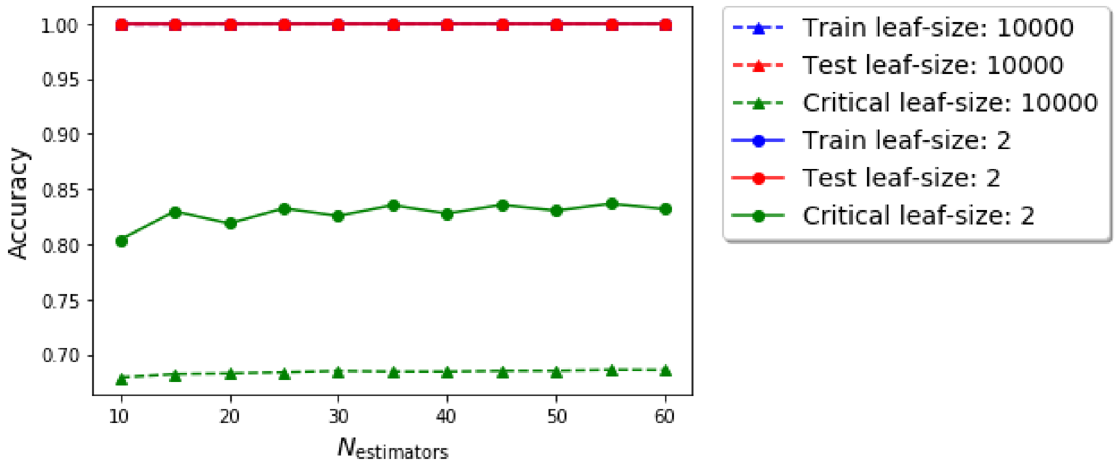
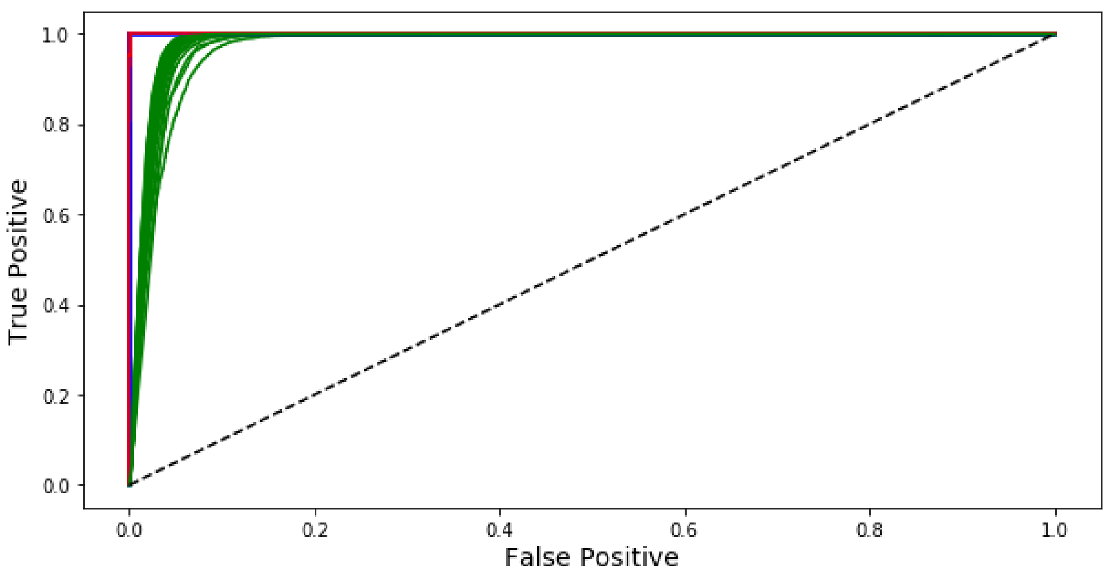
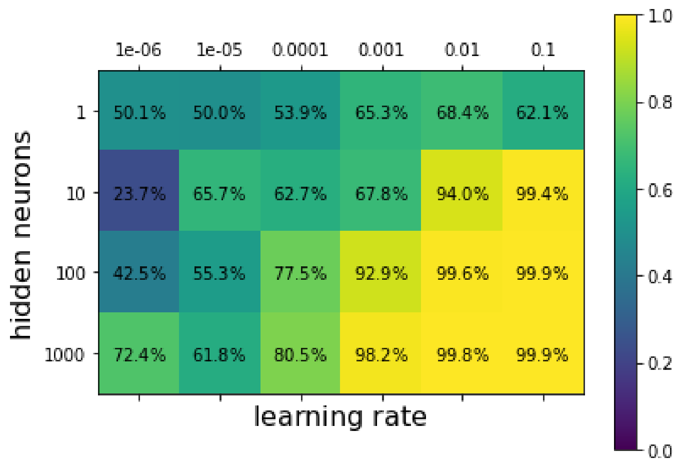
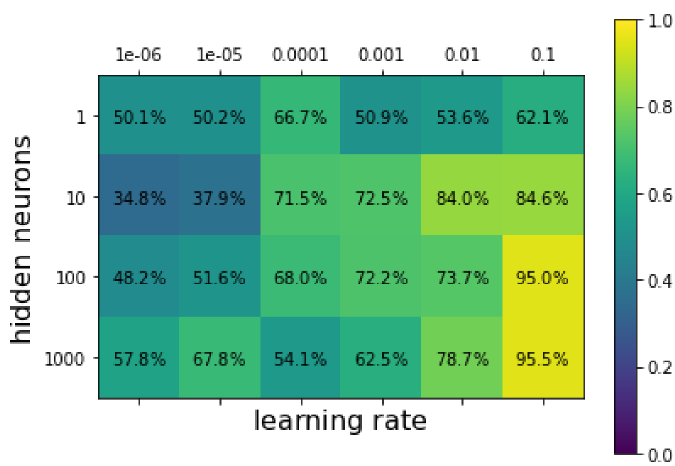




0.0.5 Classifying the Ising Model Phase Using Neural Networks





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