Project_on_Machine_Learning

June 26, 2018

1 Project on Machine Learning

- Ising Model
- Metha et al, arXiv 1803.08823 accompanied by a Jupyter notebook.
- Phases
  - Ordered
  - Critical
  - Disordered

2 Linear Regression

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

2.1 Ridge Regression

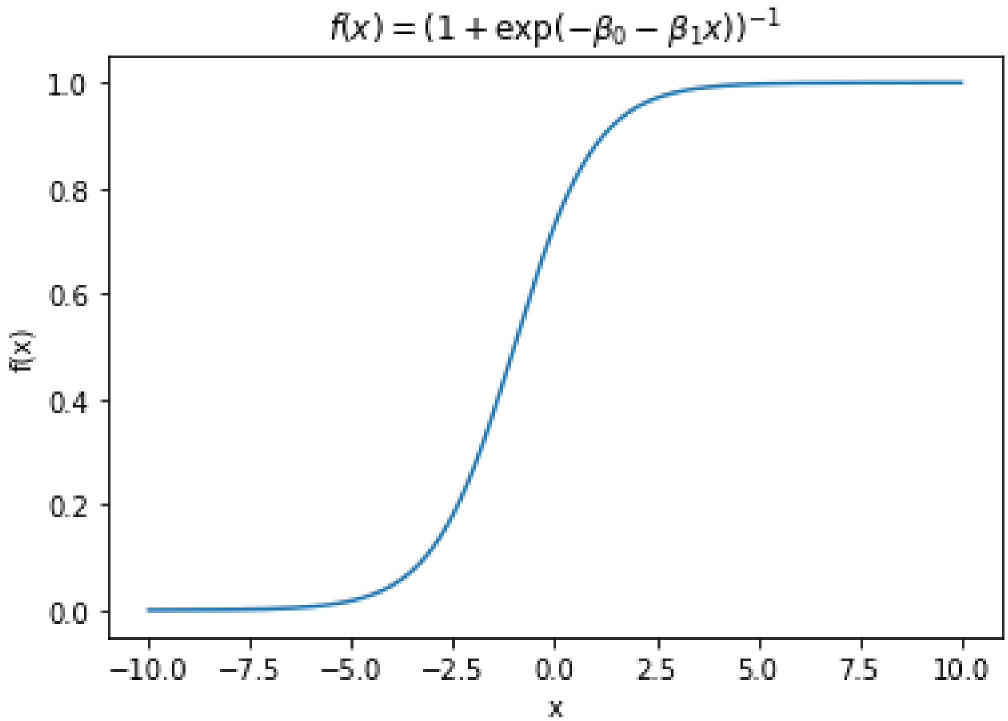
- L_2-regularization: $\boldsymbol{y} = \boldsymbol{X}\boldsymbol{\beta} + \alpha \sum_{i=1}^{m} \beta_i^2$
- $\boldsymbol{\beta}_{\text{Ridge}} = \underset{\boldsymbol{\beta}}{\operatorname{argmin}} \left(\left| \boldsymbol{X}\boldsymbol{\beta} - \boldsymbol{y} \right|^2 + \alpha \left| \boldsymbol{\beta}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

2.2 Lasso Regression

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

3 Logistic Regression

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



The idea with the binary logistic regression is to find the probability for a stochastic variable X to be part of some category Y, this is just a joint probability $P(Y|X)$. In terms of regression terminology Y would be the response and X the explanatory variable. X can be a data-point and the categories can be expressed as $Y = \{0, 1\}$. Since we work with data-points it is convenient to index them as

$$X \to X_i$$

$$Y \to Y_i = \{0, 1\}$$

The probabilites can then be expressed as

$$f(Y_i = 1|\boldsymbol{X}_i, \boldsymbol{w}) = \frac{1}{1 + \exp(-\boldsymbol{X}_i^T\boldsymbol{w})}$$

$$f(Y_i = 0|\boldsymbol{X}_i, \boldsymbol{w}) = 1 - f(Y_i = 1|\boldsymbol{X}_i)$$

The problem addressed is simply a dataset with points $\boldsymbol{X}_i$ and binary labels $Y_i \in \{0, 1\}$. Considering drawing datapoints independently the likelihood of seing some data $D_i = \{(Y_i, \boldsymbol{X}_i)\}$ is

$$P(D_i|\boldsymbol{w}) = \prod_{i=1}^{n} \left[f\left(\boldsymbol{X}_i^T\boldsymbol{w}\right)\right]^{Y_i} \left[1 - f\left(\boldsymbol{X}_i^T\boldsymbol{w}\right)\right]^{1-Y_i},$$

and the maximum likelihood estimator(MLE) is defined as the set of parameters which maximizes the log-likelihood(log of above function). The expression for $\boldsymbol{w}$ is

$$\boldsymbol{w}_{\text{MLE}} = \underset{w}{\operatorname{argmax}} \sum_{i=1}^{n} \left[y_i \log \left(f \left(\boldsymbol{X}_i^T \boldsymbol{w} \right) \right) + (1 - Y_i) \log \left(1 - f \left(\boldsymbol{X}_i^T \boldsymbol{w} \right) \right) \right].$$

The cost is just the negative log-likelihood and is known as the cross-entropy in statistics. The expression is

$$C(\boldsymbol{w}) = -\sum_{i=1}^{n} \left[Y_i \log \left(f \left(\boldsymbol{X}_i^T \boldsymbol{w} \right) \right) + (1 - Y_i) \log \left(1 - f \left(\boldsymbol{X}_i^T \boldsymbol{w} \right) \right) \right].$$

The cross-entropy is convex by the second-derivative test(with respect to parameters $\boldsymbol{w}$) meaning a simple minimization gives the global minimum. The equation is

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

This is a transcendental equation for $\boldsymbol{w}$ which has to be solved numerically by some numerical optimization scheme such as gradient descent or some Quasi-Newton method.

3.0.1 Random Forest Algorithm

A random forest is, in the context of data science, a family of randomized tree-based classifier decision trees. The basic structure of the decision tree is formed as a series of questions which partition the data. The random forest is then made by creating an ensemble of such trees with a randomization procedure, some of these are - **Bagging**: Reduce variance by creating several subset of data from sample choosen in random with replacement. Each subset is then trained giving in total an ensemble of different models. - **Feature Bagging**: Reduces correlations between decision trees by creating several subset of the features at each split of the tree. - **Extremized Random Forest**: Prevent overfitting and reduce correllations, but reduce predictive power by combining ordinary and feature bagging with an extreme randomization procedure where the splitting is done at random instead of optimal criteria.

3.0.2 Neural Networks

A neural network is essentially just a linear transformation that weights the values of different inputs by a non-linear activation function and is a supervised learning method. The basic idea is with the so-called neuron which just represents a node (or element) in the network. Then, stack a number of these in to form a layer. The first layer is called the input and is represented by an $n \times d$ matrix

$$\boldsymbol{x} = \begin{pmatrix} x_{11} & \dots & x_{1d} \\ \vdots & \ddots & \vdots \\ x_{d1} & \dots & x_{nd} \end{pmatrix},$$

with the node being the elements in $\boldsymbol{x}$. A number of layers with sizes $(n_2, \dots, n_m)$ (number of nodes) are then laid between the input and the output, these are known as hidden layers. The weighting is then represented as a set of neuron-specific matrices

$$\{\boldsymbol{w}\}_{l=1}^{m} = \left(\boldsymbol{w}^{(1)}, \dots, \boldsymbol{w}^{(m)} \right).$$

The transformation in layer l is then specified by $\boldsymbol{w}^{(l)}$ and the output serves as the input to the next layer. The last transformation gives the output. It is also common to introduce a bias $b^{(l)}$ meaning the transformation $z^{(l)}$ for layer l is actually

$$z^{(l)} = \boldsymbol{w}^{(l)} \cdot \boldsymbol{x} + b^{(l)}$$

The shape of $\boldsymbol{w}^{(l)}$ is determined by the layer. $\boldsymbol{w}^{(1)}$ is a $(d \times n_1)$ matrix where n_i is the number of nodes in the first hidden layer and $\boldsymbol{w}^{(2)}$ has shape $n_1 \times n_2$ and so on. In general the shape of $\boldsymbol{w}^{(i)}$ is $n_i \times n_{i+1}$ where $n_1 = d$.

With the neural-network model at hand the weights and the biases have to be determined. The procedure is the same as previously, define the cost function and minimize. We may write that given the data-point $(\boldsymbol{x}_i, y_i)$ the neural network makes a prediction $\hat{y}_i(\boldsymbol{w}, \boldsymbol{b})$.

Backpropagation In order to actually minimize the cost function a so-called backpropagation has to be made. Assuming our neural-network has - L: Number of layers - w^l_{jk}: Weight for k-th neuron in layer $l-1$ to j-th neuron in layer l - b^l_j: Bias of neuron j in layer l - a^l_j: Activation of neuron j in layer l

The activation is related by the non-linear transformation σ

$$a^l_j = \sigma\left(\sum_k w^l_{kj} a^{l-1}_k\right).$$

We define two new quantities, the linear weigthed sum

$$z^l_j = \sum_k w^l_{jk} a^{l-1}_k + b^l_j$$

and the error of neuron j

$$\Delta^L_j = \frac{\partial E}{\partial z^L_j}.$$

The error of neuron j in layer l is equivalently

$$\Delta^l_j = \frac{\partial E}{\partial z^l_j} = \frac{\partial E}{\partial a^l_j}\frac{\partial \sigma}{\partial z^l_j},$$

by the chain rule. The error terms can also be expressed as

$$\Delta^l_j = \frac{\partial E}{\partial z^l_j} = \frac{\partial E}{\partial b^l_j}\frac{\partial b^l_j}{\partial z^l_j} = \frac{\partial E}{\partial b^l_j},$$

since

$$\frac{\partial b^l_j}{\partial z^l_j} = 1.$$

The activation transformation can be expressed with z^l_j as

$$a^l_j = \sigma\left(z^l_j\right).$$

A third expression of the error is

$$\Delta_j^L = \frac{\partial E}{\partial z_j^l} = \sum_k \frac{\partial E}{\partial z_k^{l+1}} \frac{\partial z_k^{l+1}}{\partial z_j^l} = \sum_k \Delta_k^{l+1} \frac{\partial z_k^{l+1}}{\partial z_j^l} = \left(\sum_k \Delta_k^{l+1} w_{kj}^{l+1} \right) \frac{\partial \sigma}{\partial z_j^l}.$$

The final expression involved is the derivative with respect to w_{jk}^l,

$$\frac{\partial E}{\partial w_{jk}^l} = \frac{\partial E}{\partial z_j^l} \frac{\partial z_j^l}{\partial w_{jk}^l} = \Delta_j^l a_k^{l-1}.$$

Combining these algorithms the backpropagation algorithm is 1. **Activation at input layer**: Calculate activations a_j^l of all neurons in the input layer. 2. **Feedforward**: Compute z^l and a^l for all subsequent layers. 3. **Error at output**: Calculate error in output layer with first expression for Δ_j^l. 4. **Backpropagate**: Use third expression for Δ_j^l to calculate Δ_j^l for all layers. 5. **Calculate Gradient**: Calculate $\frac{\partial E}{\partial b_j^l}$ and $\frac{\partial E}{\partial w_{jk}^l}$.

With the efficient forward sweep through the network and one backpropagation the gradient is readily calculated and the minimization can be done with the same methods as with the logistic regression scheme.

Cost function We have yet to mention the actual cost function with the neural network. These are the same as introduced with the linear regression schemes, that is either the mean-square error

$$E(\boldsymbol{w}, \boldsymbol{b}) = \frac{1}{N} \sum_i \left(y_i - \hat{y}_i(\boldsymbol{w}, \boldsymbol{b}) \right)^2,$$

and the mean absolute error(L_1-norm)

$$E(\boldsymbol{w}, \boldsymbol{b}) = \frac{1}{N} \sum_i \left| y_i - \hat{y}_i(\boldsymbol{w}, \boldsymbol{b}) \right|.$$

The cross-entropy

$$C(\boldsymbol{w}) = -\sum_{i=1}^{n} \left[y_i \log\left(\hat{y}_i(\boldsymbol{w})\right) + (1 - y_i) \log\left(1 - \hat{y}_i(\boldsymbol{w})\right) \right].$$

can still be used if the data is categorical. More generally if y can take more values, $y \in 0, 1, \ldots, M-1$, we may define

$$y_{im} = \begin{cases} 1, & y_i = m \\ 0, & \text{else} \end{cases},$$

and the categorical cross-entropy is

$$E(\boldsymbol{w}) = -\sum_{i=1}^{n} \sum_{m=0}^{M-1} \left(y_{im} \log\left(\hat{y}_{im}(\boldsymbol{w})\right) + (1 - y_{im} \log\left(1 - \hat{y}_{im}(\boldsymbol{w})\right) \right).$$

Depending on the data one of these cost functions can be used in the backpropagation algorithm and the training can proceed.

3.1 Implementation and Results

3.1.1 Estimating the Coupling Constant of the 1D Ising Model

In estimating the coupling constant we use data generated with $J = 1$ and use the linear regression schemes presented.

In order to use linear regression with the Ising model we assume the model (without any prior knowledge) the all-to-all Ising model

$$E^{(i)} = -\sum_{kl}^{N} J_{kl} s_k^{(i)} s_l^{(i)},$$

with the J_{kl} being the coupling strengths we wish to learn. The index i represents a sample point. This equation can be rewritten as the matrix equation

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

with $\boldsymbol{X}^{(i)}$ representing the two-body interactions

$$\left\{ s_k^{(i)}, s_l^{(i)} \right\}_{k,l=1}^{N}.$$

This is the exact linear regression presented earlier.

Let us first generate $N = 10000$ states of a system of length $L = 40$ and divide the data into a training set and test set. This is to test the performance of the algorithm on a set it has not seen before (hence the test set).

```
In [51]: import numpy as np
         import scipy.sparse as sp

         np.random.seed(12)

         def ising_energies(states, L):
             """ Calculate energy """
             J = np.zeros((L,L),)
             for i in range(L):
                 J[i, (i+1)%L] -= 1.0
             # end for

             return np.einsum('...i,ij,...j->...', states, J, states)
         # end function ising_energies

         L= 40 # system size
         N = 10000 # number of states

         # generate Ising states
         states = np.random.choice([-1,1], size=(N, L))

         energies = ising_energies(states, L)
```

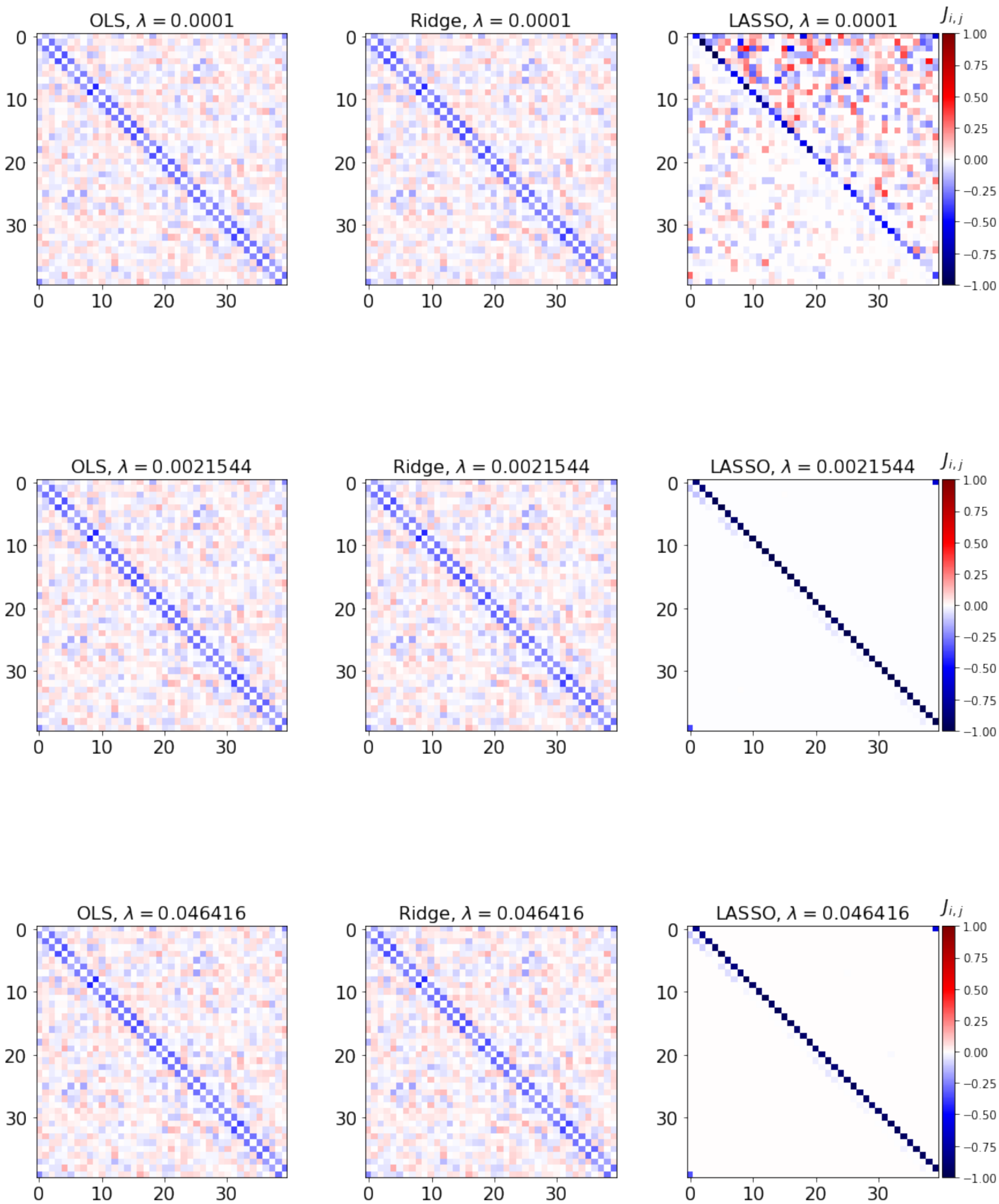
```
# reshape states into a single index (i,j) --> p
states = np.einsum('...i,...j->...ij', states, states)
shape = states.shape
states = states.reshape((shape[0], shape[1]*shape[2]))

# build final set
data = [states, energies]

n_samples = 400 # number of samples

# define training and test data
X_train=data[0][:n_samples]
Y_train=data[1][:n_samples] #+ np.random.normal(0,4.0,size=X_train.shape[0])
X_test=data[0][n_samples:3*n_samples//2]
Y_test=data[1][n_samples:3*n_samples//2] #+ np.random.normal(0,4.0,size=X_test.shape[0]
```

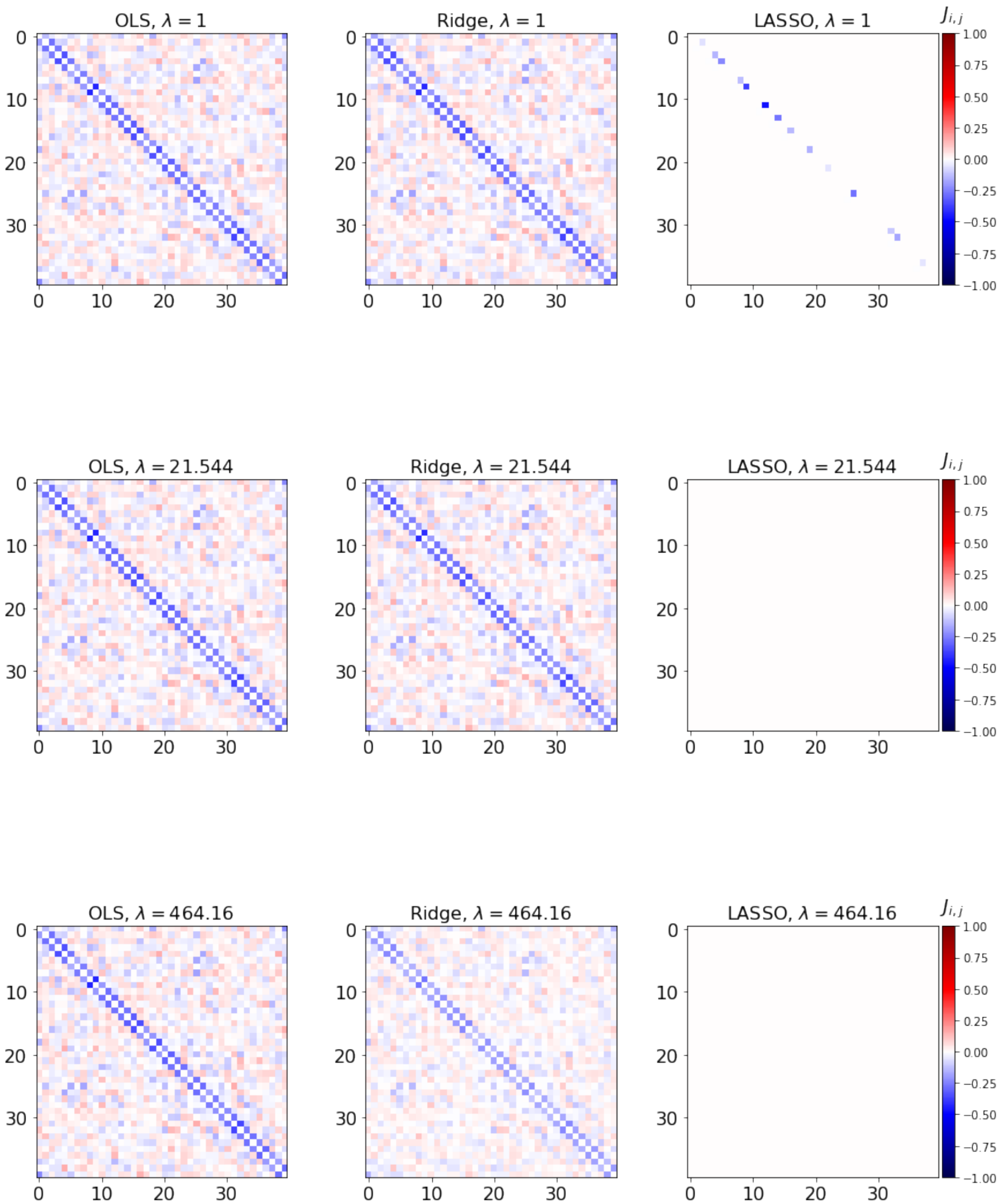
Now we can start to apply the least-squares, ridge regression and LASSO methods using the scikit-learn package.

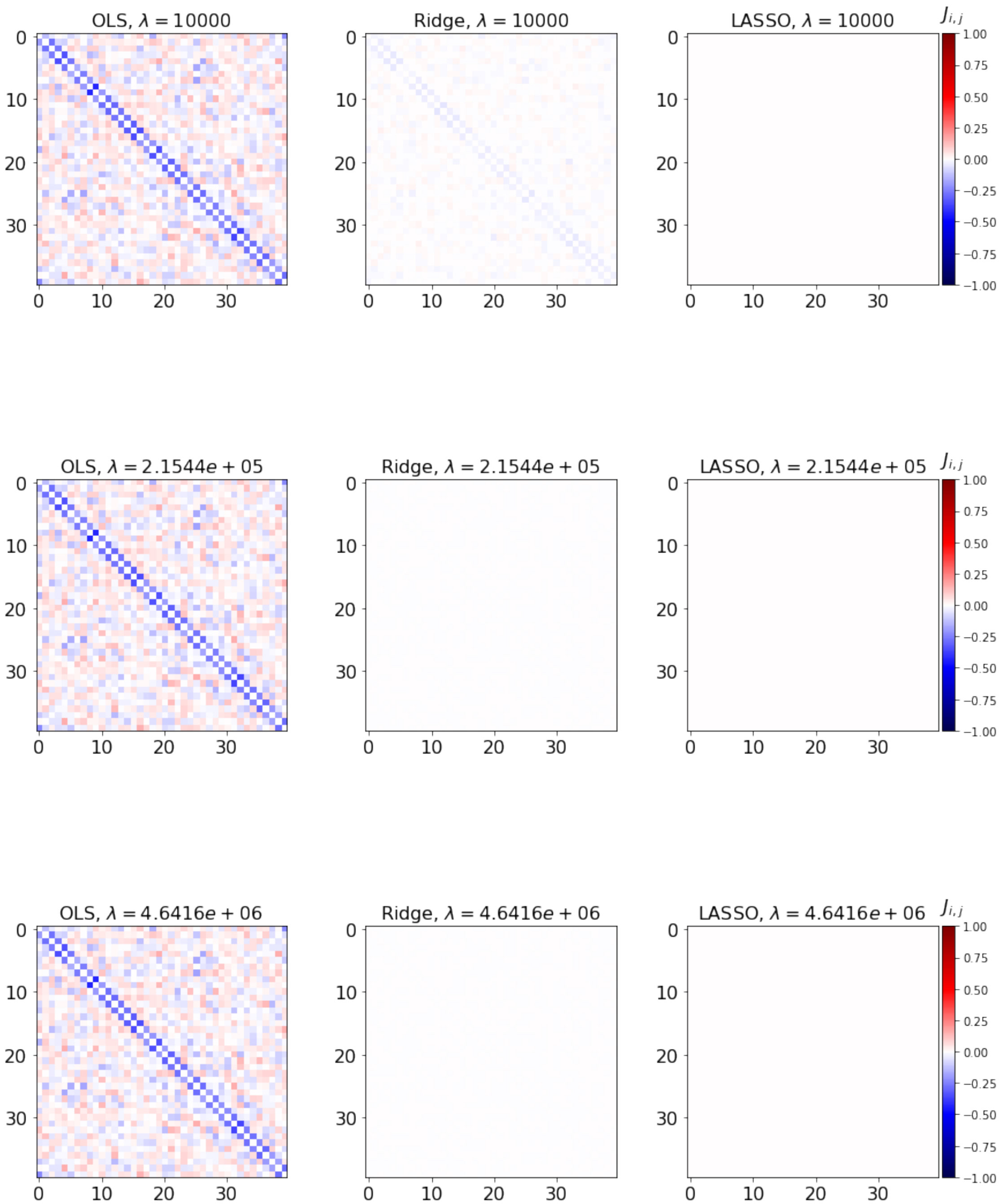
```
In [52]: from sklearn import linear_model
         import matplotlib.pyplot as plt
         from mpl_toolkits.axes_grid1 import make_axes_locatable

         def make_plot(coefs, L, lamdas, titles=['OLS', 'Ridge', 'LASSO']):
             """ plot results """

             cmap_args = dict(vmin=-1., vmax=1., cmap='seismic')
             for l,lamda in enumerate(lamdas):
                 fig, ax = plt.subplots(nrows=1, ncols=len(coefs))
                 for i,coeff in enumerate(coefs):
                     J = np.array(coeff[l]).reshape((L,L))
                     im = ax[i].imshow(J, **cmap_args)
                     ax[i].set_title(titles[i] + ", $\\lambda=%.5g$" % lamda, fontsize=16)
                     ax[i].tick_params(labelsize=16)
                 # end forl

                 divider = make_axes_locatable(ax[2])
                 cax = divider.append_axes("right", size="5%", pad=0.05)
                 cbar = fig.colorbar(im, cax=cax)

                 cbar.set_label('$J_{i,j}$', labelpad=-40, y=1.12, fontsize=16, rotation=0)
                 fig.subplots_adjust(right=2.0)
             # end fori

             plt.show()
         # end function make_plot

         def apply_method(model, x_train, y_train, x_test, y_test, lamda=None):
```

```
    """ apply model, return weights and performance score """

    # set regularization parameter if given
    if lamda:
        model.set_params(alpha=lamda)
    # end if

    # run fitting and store weights
    model.fit(x_train, y_train)

    return model.coef_, model.score(x_train, y_train), model.score(x_test, y_test)
# end function apply_method

def grab_axis(nested_list, j=0):
    """ slice list and return axis j """
    return [[i[j] for i in r] for r in nested_list]
# end function grab_axis_i

# list for results
results = []

# regularization parameters
lamdas = np.logspace(-4,8,10)

least_squares_results = apply_method(linear_model.LinearRegression(), X_train, Y_train,
results.append([least_squares_results for r in range(len(lamdas))])

for rl in [linear_model.Ridge(), linear_model.Lasso()]:
    tmp_res = []
    for lamda in lamdas:
        tmp_res.append(apply_method(rl, X_train, Y_train, X_test, Y_test, lamda))
    # end for lamda
    results.append(tmp_res)
# end for rl

make_plot(grab_axis(results,0), L, lamdas)
```

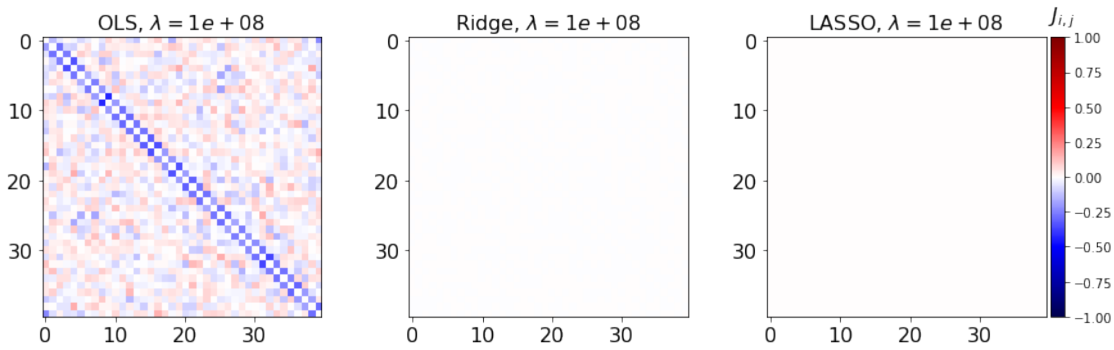
```
/usr/local/lib/python3.6/dist-packages/sklearn/linear_model/coordinate_descent.py:491: Convergen
  ConvergenceWarning)
```


OLS, $\lambda = 0.0001$
Ridge, $\lambda = 0.0001$
LASSO, $\lambda = 0.0001$
OLS, $\lambda = 0.0021544$
Ridge, $\lambda = 0.0021544$
LASSO, $\lambda = 0.0021544$
OLS, $\lambda = 0.046416$
Ridge, $\lambda = 0.046416$
LASSO, $\lambda = 0.046416$
$J_{i,j}$
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
0
10
20
30


OLS, $\lambda = 1$
Ridge, $\lambda = 1$
LASSO, $\lambda = 1$
OLS, $\lambda = 21.544$
Ridge, $\lambda = 21.544$
LASSO, $\lambda = 21.544$
OLS, $\lambda = 464.16$
Ridge, $\lambda = 464.16$
LASSO, $\lambda = 464.16$
$J_{i,j}$
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00
0
10
20
30

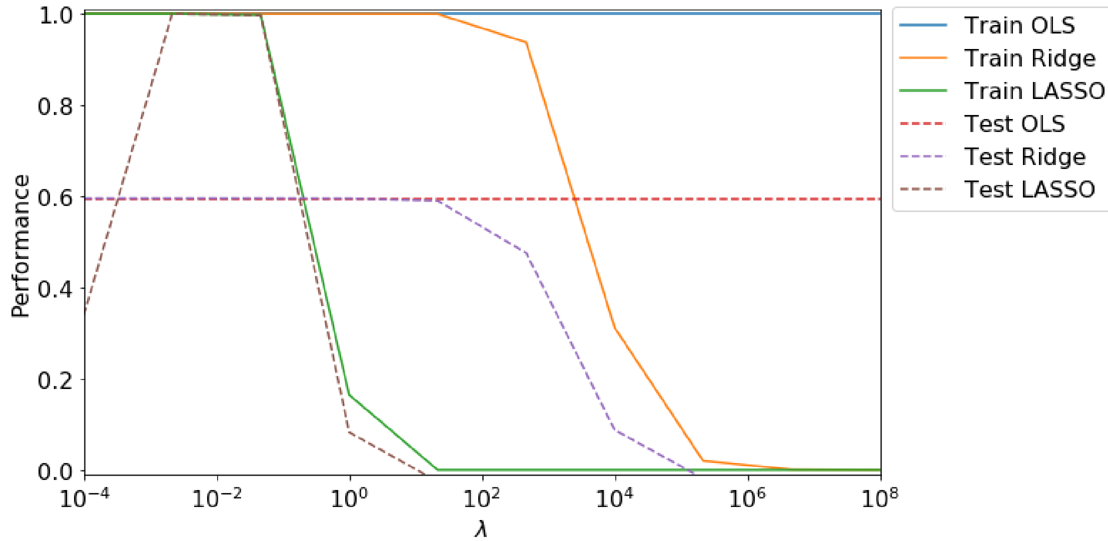


OLS, λ = 10000
Ridge, λ = 10000
LASSO, λ = 10000
OLS, λ = 2.1544e + 05
Ridge, λ = 2.1544e + 05
LASSO, λ = 2.1544e + 05
OLS, λ = 4.6416e + 06
Ridge, λ = 4.6416e + 06
LASSO, λ = 4.6416e + 06
J_{i,j}



In order to actually see the performance we plot the training and test errors.

```
In [53]: def plot_errors(train_errors, test_errors, lamdas, titles=["OLS", "Ridge", "LASSO"]):
             """ plot in-sample and out-of-sample errors, aka performance"""
             for i,trnerr in enumerate(train_errors):
                 plt.semilogx(lamdas, trnerr, label="Train " + titles[i])
             # end fori

             for i,tsterr in enumerate(test_errors):
                 plt.semilogx(lamdas, tsterr, '--', label="Test " + titles[i])
             # end fori

             fig = plt.gcf()
             fig.set_size_inches(10.0, 6.0)

             plt.legend(bbox_to_anchor=(1.0, 1.03),fontsize=16)
             plt.ylim([-0.01, 1.01])
             plt.xlim([min(lamdas), max(lamdas)])
             plt.xlabel(r'$\lambda$',fontsize=16)
             plt.ylabel('Performance',fontsize=16)
             plt.tick_params(labelsize=16)
             plt.show()
         # end function plot_errors

         plot_errors(grab_axis(results, 1), grab_axis(results, 2), lamdas)
```



From the plot of the linear fit we can see that all methods seemingly fits the data well, however the performance plot indicates that all three methods overfit the data. With the OLS the overfitting cannot be fixed since no regularization is involved. For the Ridge method the overfitting is less as λ is increased, however the fit is worse. For the LASSO method the same applies, but the overfitting is much less and the performance is actually indicates that the fit is spot-on for $\lambda \approx 10^{-2}$. For this λ we see that J only contains nearest-neghbour terms which is how the original data was generated.

3.1.2 Determine the Phase of the Two-Dimensional Ising Model

The binary logistic regression can be used to determine the phase of the two-dimensional Ising model. The Hamiltonian is given by

$$H = -J \sum_{<kl>} s_k s_l,$$

with the k and l indices running over the nearest neighbors on a 2D square lattice. J is the energy scale. It has been proved by Onsager that the system undergoas a phase transition in between the ordered and disordered state at a critical temperature

$$\frac{T_c}{J} = \frac{2}{\log\left(1+\sqrt{2}\right)} \approx 2.26.$$

The question is then, can we train a classifier to distinguish the two phases of the Ising model. The problem is then a binary classification since we have two categories, namely ordered and unordered. With - Ordered: $\frac{T}{J} < 2.0$ - Near-critical: $2.0 \le \frac{T}{J} \le 2.5$ - Disorderd: $\frac{T}{J} \ge 2.0$

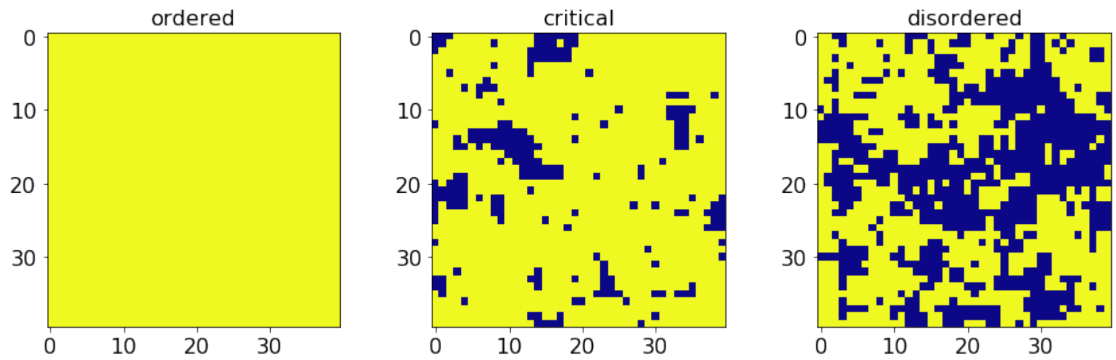
Firstly we need some data. We use the data provided by the mentioned article. These are data of 10^4 states from Monte-Carlo simulations on a $L \times L$ square lattice with $L = 40$.

```
In [54]: import pickle
         import os
         from sklearn.model_selection import train_test_split
```

```python
def plot_2D_states(states, L, titles=["ordered", "critical", "disordered"]):
    """visualize states"""
    cmap_args = dict(cmap='plasma_r')

    fig, ax = plt.subplots(nrows=1, ncols=len(states))

    for i,s in enumerate(states):
        ax[i].imshow(s.reshape(L,L), **cmap_args)
        ax[i].set_title(titles[i], fontsize=16)
        ax[i].tick_params(labelsize=16)
    # end fors

    fig.subplots_adjust(right=2.0)

    plt.show()
# end function plot_2D_states

# shuffle generator seed
np.random.seed()

# Ising parameters
L = 40
J = -1.0
T = np.linspace(0.25,4.0,16)
T_c = 2.26

# define regression parameters
num_classes = 2
train_test_ratio = 0.5

# load data (all of it)
data_path = "IsingData/"
data = pickle.load(open(data_path + "Ising2DFM_reSample_L40_T=All.pkl", 'rb'))
data = np.unpackbits(data).reshape(-1, 1600)
data = data.astype(np.int32)
data[np.where(data==0)] = -1

# load labels (all of it)
labels = pickle.load(open(data_path + "Ising2DFM_reSample_L40_T=All_labels.pkl", "rb"))

# divide data into ordered, critical and disordered
start1 = 0
end1 = 70000
end2 = 100000
end3 = -1
X_ordered=data[start1:end1,:]
Y_ordered=labels[start1:end1]
```

```python
X_critical=data[end1:end2,:]
Y_critical=labels[end1:end2]

X_disordered=data[end2:end3,:]
Y_disordered=labels[end2:end3]

del data,labels

# define training and test
Xt=np.concatenate((X_ordered,X_disordered))
Yt=np.concatenate((Y_ordered,Y_disordered))

# pick at random to create training and test
X_train, X_test, Y_train, Y_test = train_test_split(Xt, Yt, train_size=train_test_ratio

# create full data set
X = np.concatenate((X_critical,Xt))
Y = np.concatenate((Y_critical,Yt))

print('X_train shape:', X_train.shape)
print('Y_train shape:', Y_train.shape)
print()
print(X_train.shape[0], 'train samples')
print(X_critical.shape[0], 'critical samples')
print(X_test.shape[0], 'test samples')

# plot data
plot_2D_states([X_ordered[int((end1-start1)/2)],
                X_critical[int((end2-end1)/2)],
                X_disordered[int((end3-end2)/2)]], L)
```

```
/usr/local/lib/python3.6/dist-packages/sklearn/model_selection/_split.py:2026: FutureWarning: Fr
  FutureWarning)


X_train shape: (64999, 1600)
Y_train shape: (64999,)

64999 train samples
30000 critical samples
65000 test samples
```



Now that we have the data, the regression can be applied.

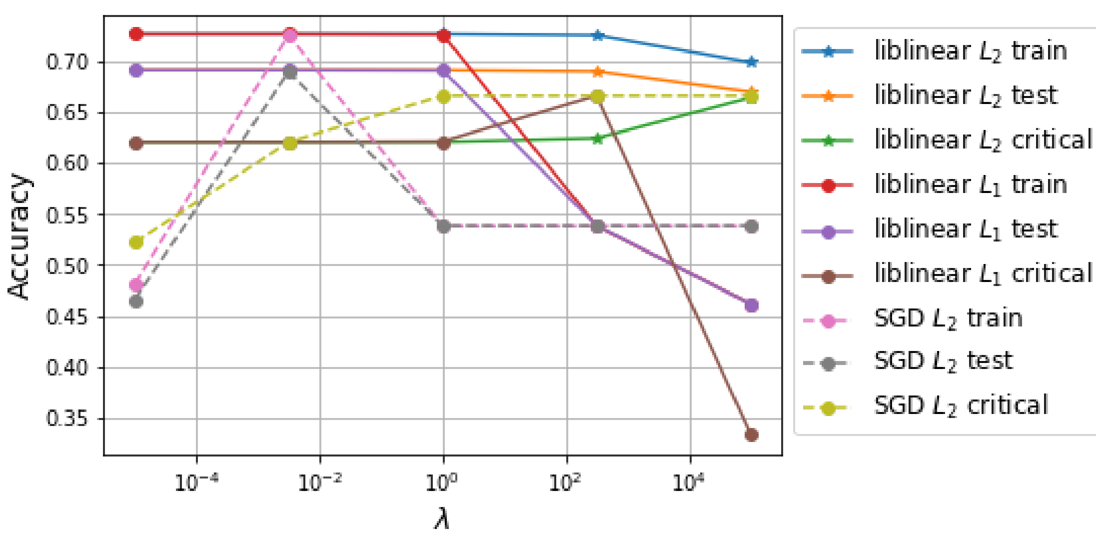
```
In [57]: from sklearn import linear_model

         # set regularization parameters
         lamdas = np.logspace(-5,5,5)

         # preallocate data
         train_accuracy=np.zeros(lamdas.shape,np.float64)
         test_accuracy=np.zeros(lamdas.shape,np.float64)
         critical_accuracy=np.zeros(lamdas.shape,np.float64)

         train_accuracy_l1=np.zeros(lamdas.shape,np.float64)
         test_accuracy_l1=np.zeros(lamdas.shape,np.float64)
         critical_accuracy_l1=np.zeros(lamdas.shape,np.float64)

         train_accuracy_SGD=np.zeros(lamdas.shape,np.float64)
         test_accuracy_SGD=np.zeros(lamdas.shape,np.float64)
         critical_accuracy_SGD=np.zeros(lamdas.shape,np.float64)

         train_preds = []
         test_preds = []
         critical_preds = []

         train_preds_l1 = []
         test_preds_l1 = []
         critical_preds_l1 = []

         train_preds_SGD = []
         test_preds_SGD = []
         critical_preds_SGD = []

         print('accuracy: train, test, critical')
         for i,lamda in enumerate(lamdas):
             # perform liblinear based logistic regression
```

```
        logreg = linear_model.LogisticRegression(C=1./lamda, random_state=1, verbose=0, max
        logreg.fit(X_train, Y_train)
        train_accuracy[i] = logreg.score(X_train, Y_train)
        test_accuracy[i] = logreg.score(X_test, Y_test)
        critical_accuracy[i] = logreg.score(X_critical, Y_critical)

        train_preds.append(logreg.predict_proba(X_train)[:,0])
        test_preds.append(logreg.predict_proba(X_test)[:,0])
        critical_preds.append(logreg.predict_proba(X_critical)[:,0])

        print('liblin: %0.4f, %0.4f, %0.4f' % (train_accuracy[i],test_accuracy[i],critical_

        # perform liblinear with L1-norm based logistic regression
        logreg_l1 = linear_model.LogisticRegression(penalty='l1', C=1./lamda, random_state=
                                                    max_iter=1e3, tol=1e-5)
        logreg_l1.fit(X_train, Y_train)
        train_accuracy_l1[i] = logreg_l1.score(X_train, Y_train)
        test_accuracy_l1[i] = logreg_l1.score(X_test, Y_test)
        critical_accuracy_l1[i] = logreg_l1.score(X_critical, Y_critical)

        train_preds_l1.append(logreg_l1.predict_proba(X_train)[:,0])
        test_preds_l1.append(logreg_l1.predict_proba(X_test)[:,0])
        critical_preds_l1.append(logreg_l1.predict_proba(X_critical)[:,0])

        print('liblinl1: %0.4f, %0.4f, %0.4f' % (train_accuracy_l1[i],test_accuracy_l1[i],c

        # perform SGD-based logistic regression
        logreg_SGD = linear_model.SGDClassifier(loss='log', penalty='l2', alpha=lamda, max_
                                                shuffle=True, random_state=1, learning_rate
        logreg_SGD.fit(X_train, Y_train)
        train_accuracy_SGD[i] = logreg_SGD.score(X_train, Y_train)
        test_accuracy_SGD[i] = logreg_SGD.score(X_test, Y_test)
        critical_accuracy_SGD[i] = logreg_SGD.score(X_critical, Y_critical)

        train_preds_SGD.append(logreg_SGD.predict_proba(X_train)[:,0])
        test_preds_SGD.append(logreg_SGD.predict_proba(X_test)[:,0])
        critical_preds_SGD.append(logreg_SGD.predict_proba(X_critical)[:,0])

        print('SGD: %0.4f, %0.4f, %0.4f' % (train_accuracy_SGD[i],test_accuracy_SGD[i],crit
    # end fori
```

```
accuracy: train, test, critical
liblin: 0.7272, 0.6917, 0.6209
liblinl1: 0.7272, 0.6917, 0.6209
SGD: 0.4811, 0.4658, 0.5219
liblin: 0.7272, 0.6917, 0.6209
liblinl1: 0.7272, 0.6917, 0.6209
SGD: 0.7259, 0.6897, 0.6208
```

```
liblin: 0.7272, 0.6917, 0.6209
liblinl1: 0.7269, 0.6913, 0.6214
SGD: 0.5383, 0.5387, 0.6667
liblin: 0.7260, 0.6904, 0.6246
liblinl1: 0.5383, 0.5386, 0.6667
SGD: 0.5383, 0.5386, 0.6667
liblin: 0.6992, 0.6701, 0.6647
liblinl1: 0.4617, 0.4614, 0.3333
SGD: 0.5383, 0.5386, 0.6667
```

In [58]:
```
plt.semilogx(lamdas, train_accuracy, "*-", label='liblinear $L_2$ train')
plt.semilogx(lamdas, test_accuracy, "*-", label='liblinear $L_2$ test')
plt.semilogx(lamdas, critical_accuracy, "*-", label='liblinear $L_2$ critical')

plt.semilogx(lamdas, train_accuracy_l1, "o-", label='liblinear $L_1$ train')
plt.semilogx(lamdas, test_accuracy_l1, "o-", label='liblinear $L_1$ test')
plt.semilogx(lamdas, critical_accuracy_l1, "o-", label='liblinear $L_1$ critical')

plt.semilogx(lamdas, train_accuracy_SGD, "o--", label='SGD $L_2$ train')
plt.semilogx(lamdas, test_accuracy_SGD, "o--", label='SGD $L_2$ test')
plt.semilogx(lamdas, critical_accuracy_SGD, "o--", label='SGD $L_2$ critical')

plt.grid()
plt.ylabel("Accuracy", fontsize=14)
plt.xlabel("$\\lambda$", fontsize=14)
plt.legend(bbox_to_anchor=(1.0, 1.0), fontsize=12)

plt.show()
```

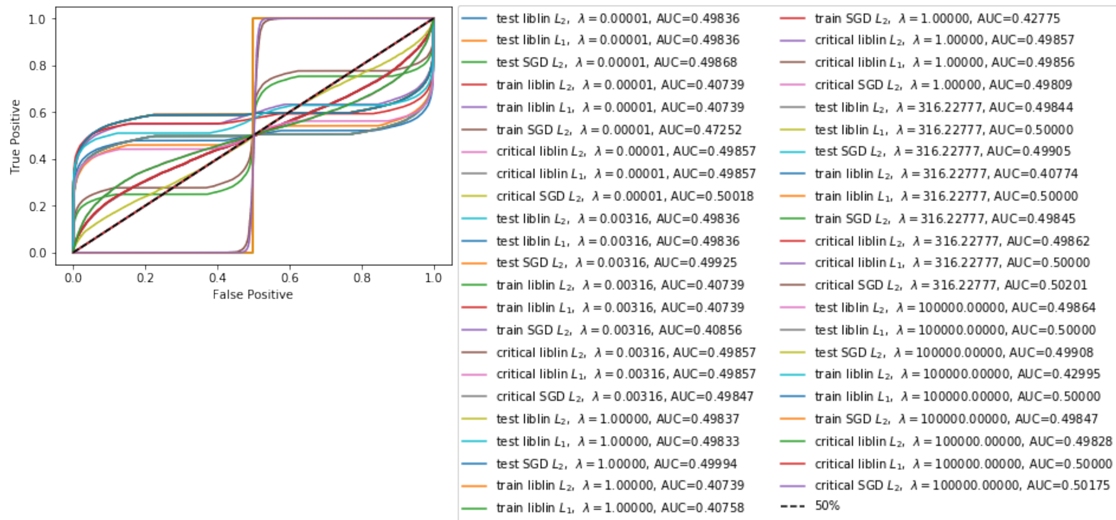


We can immedietly see a degree og overfitting and the performance of the optimizer depends on the regularization strength λ. There is also a sweet spot similarly to the logistic regression case for the SGD. Here it is around $\lambda \approx 10^{-1}$. The phase is also difficult to predict around the critical region. For the liblinear, lbfgs and saga the performance only drops as λ is increased much (above around 10^3). This just indicates that the regularisation strength does not have much impact.

We can also make a receiver operator characteristic (ROC) to further diagonize the classifier.

```
In [59]: from sklearn.metrics import roc_curve, roc_auc_score

         for i,lamda in enumerate(lamdas):
             logreg_tpr, logreg_fpr, _ = roc_curve(Y_test, test_preds[i])
             logreg_l1_tpr, logreg_l1_fpr, _ = roc_curve(Y_test, test_preds_l1[i])
             logreg_SGD_tpr, logreg_SGD_fpr, _ = roc_curve(Y_test, test_preds_SGD[i])

             logreg_auc = roc_auc_score(Y_test, test_preds[i])
             logreg_l1_auc = roc_auc_score(Y_test, test_preds_l1[i])
             logreg_SGD_auc = roc_auc_score(Y_test, test_preds_SGD[i])

             plt.plot(logreg_fpr, logreg_tpr, label="test liblin $L_2$,  $\lambda=%.5f$, AUC=$%.
             plt.plot(logreg_l1_fpr, logreg_l1_tpr, label="test liblin $L_1$,  $\lambda=%.5f$, A
             plt.plot(logreg_SGD_fpr, logreg_SGD_tpr, label="test SGD $L_2$,  $\lambda=%.5f$, AU

             logreg_tpr, logreg_fpr, _ = roc_curve(Y_train, train_preds[i])
             logreg_l1_tpr, logreg_l1_fpr, _ = roc_curve(Y_train, train_preds_l1[i])
             logreg_SGD_tpr, logreg_SGD_fpr, _ = roc_curve(Y_train, train_preds_SGD[i])

             logreg_auc = roc_auc_score(Y_train, train_preds[i])
             logreg_l1_auc = roc_auc_score(Y_train, train_preds_l1[i])
             logreg_SGD_auc = roc_auc_score(Y_train, train_preds_SGD[i])

             plt.plot(logreg_fpr, logreg_tpr, label="train liblin $L_2$,  $\lambda=%.5f$, AUC=$%
             plt.plot(logreg_l1_fpr, logreg_l1_tpr, label="train liblin $L_1$,  $\lambda=%.5f$,
             plt.plot(logreg_SGD_fpr, logreg_SGD_tpr, label="train SGD $L_2$,  $\lambda=%.5f$, A

             logreg_tpr, logreg_fpr, _ = roc_curve(Y_critical, critical_preds[i])
             logreg_l1_tpr, logreg_l1_fpr, _ = roc_curve(Y_critical, critical_preds_l1[i])
             logreg_SGD_tpr, logreg_SGD_fpr, _ = roc_curve(Y_critical, critical_preds_SGD[i])

             logreg_auc = roc_auc_score(Y_critical, critical_preds[i])
             logreg_l1_auc = roc_auc_score(Y_critical, critical_preds_l1[i])
             logreg_SGD_auc = roc_auc_score(Y_critical, critical_preds_SGD[i])

             plt.plot(logreg_fpr, logreg_tpr, label="critical liblin $L_2$,  $\lambda=%.5f$, AUC
             plt.plot(logreg_l1_fpr, logreg_l1_tpr, label="critical liblin $L_1$,  $\lambda=%.5f
             plt.plot(logreg_SGD_fpr, logreg_SGD_tpr, label="critical SGD $L_2$,  $\lambda=%.5f$
         # end fori

         plt.plot((0,1), (0,1), "--k", label='50%')
```

```
plt.legend(bbox_to_anchor=(1.0, 1.027), shadow=True, fancybox=True, ncol=2)
plt.xlabel("False Positive")
plt.ylabel("True Positive")
plt.show()
```



The ROC-curve tells us how many predictions were actually correct. Essentially this means the more the graph is above the naive-guess-line (diagonal), the better since the ratio between positive and negative then favors positive. The AUC score (area under curve) gives the probability for the classifier to rank a randomly choosen positive instance higher than an equally choosen negative one.

3.1.3 Using Random Forest to Classify Phases in the Ising Model

As with the logistic regression, Random Forest algorithm can be used to determine the phases of the Ising model. We start with the ordinary out-of-bag method (ordinary bagging).

```
In [60]: # increase training set, reduce test set
         train_test_ratio = 0.8

         # pick at random to create training and test
         X_train, X_test, Y_train, Y_test = train_test_split(Xt, Yt, train_size=train_test_ratio

         print('X_train shape:', X_train.shape)
         print('Y_train shape:', Y_train.shape)
         print()
         print(X_train.shape[0], 'train samples')
         print(X_critical.shape[0], 'critical samples')
         print(X_test.shape[0], 'test samples')
```

```
/usr/local/lib/python3.6/dist-packages/sklearn/model_selection/_split.py:2026: FutureWarning: Fr
  FutureWarning)


X_train shape: (103999, 1600)
Y_train shape: (103999,)

103999 train samples
30000 critical samples
26000 test samples
```

```
In [61]: from sklearn.ensemble import RandomForestClassifier

         min_estimators = 10
         max_estimators = 61
         n_estimators = np.arange(min_estimators, max_estimators, 5)
         leaf_sizes = [2, 10000]
         n = len(n_estimators)
         m = len(leaf_sizes)

         RFC_OOB_accuracy = np.zeros((n,m))
         RFC_train_accuracy = np.zeros((n,m))
         RFC_test_accuracy = np.zeros((n,m))
         RFC_critical_accuracy = np.zeros((n,m))

         rfc_train_preds = []
         rfc_test_preds = []
         rfc_critical_preds = []

         print('train estimate test critical')
         for i in range(0,n):
             for j in range(0,m):
                 RFC = RandomForestClassifier(n_estimators=n_estimators[i], max_depth=None,
                                              min_samples_split=leaf_sizes[j], oob_score=True, r
                 RFC.fit(X_train, Y_train)

                 RFC_train_accuracy[i,j] = RFC.score(X_train, Y_train)
                 RFC_OOB_accuracy[i,j] = RFC.oob_score
                 RFC_test_accuracy[i,j] = RFC.score(X_test, Y_test)
                 RFC_critical_accuracy[i,j] = RFC.score(X_critical, Y_critical)

                 rfc_train_preds.append(RFC.predict_proba(X_train)[:,0])
                 rfc_test_preds.append(RFC.predict_proba(X_test)[:,0])
                 rfc_critical_preds.append(RFC.predict_proba(X_critical)[:,0])

                 print('n_estimators: ' + str(n_estimators[i]) + ', leaf_size: ' + str(leaf_size
                 print('liblin: %0.4f, %0.4f,  %0.4f, %0.4f \n\n' % (RFC_train_accuracy[i,j],
```

```
                                                                    RFC_OOB_accuracy[i,j],
                                                                    RFC_test_accuracy[i,j],
                                                                    RFC_critical_accuracy[i,j])
            # end forj
        # end fori
```

```
train estimate test critical


/usr/local/lib/python3.6/dist-packages/sklearn/ensemble/forest.py:453: UserWarning: Some inputs
  warn("Some inputs do not have OOB scores. "
/usr/local/lib/python3.6/dist-packages/sklearn/ensemble/forest.py:458: RuntimeWarning: invalid v
  predictions[k].sum(axis=1)[:, np.newaxis])


n_estimators: 10, leaf_size: 2
liblin: 1.0000, 1.0000,  0.9999, 0.8031


/usr/local/lib/python3.6/dist-packages/sklearn/ensemble/forest.py:453: UserWarning: Some inputs
  warn("Some inputs do not have OOB scores. "
/usr/local/lib/python3.6/dist-packages/sklearn/ensemble/forest.py:458: RuntimeWarning: invalid v
  predictions[k].sum(axis=1)[:, np.newaxis])


n_estimators: 10, leaf_size: 10000
liblin: 0.9992, 1.0000,  0.9991, 0.6778


/usr/local/lib/python3.6/dist-packages/sklearn/ensemble/forest.py:453: UserWarning: Some inputs
  warn("Some inputs do not have OOB scores. "
/usr/local/lib/python3.6/dist-packages/sklearn/ensemble/forest.py:458: RuntimeWarning: invalid v
  predictions[k].sum(axis=1)[:, np.newaxis])


n_estimators: 15, leaf_size: 2
liblin: 1.0000, 1.0000,  1.0000, 0.8309


/usr/local/lib/python3.6/dist-packages/sklearn/ensemble/forest.py:453: UserWarning: Some inputs
  warn("Some inputs do not have OOB scores. "
/usr/local/lib/python3.6/dist-packages/sklearn/ensemble/forest.py:458: RuntimeWarning: invalid v
  predictions[k].sum(axis=1)[:, np.newaxis])
```

```
n_estimators: 15, leaf_size: 10000
liblin: 0.9993, 1.0000,  0.9992, 0.6812
```

```
/usr/local/lib/python3.6/dist-packages/sklearn/ensemble/forest.py:453: UserWarning: Some inputs
  warn("Some inputs do not have OOB scores. "
/usr/local/lib/python3.6/dist-packages/sklearn/ensemble/forest.py:458: RuntimeWarning: invalid v
  predictions[k].sum(axis=1)[:, np.newaxis])
```

```
n_estimators: 20, leaf_size: 2
liblin: 1.0000, 1.0000,  1.0000, 0.8199
```

```
/usr/local/lib/python3.6/dist-packages/sklearn/ensemble/forest.py:453: UserWarning: Some inputs
  warn("Some inputs do not have OOB scores. "
/usr/local/lib/python3.6/dist-packages/sklearn/ensemble/forest.py:458: RuntimeWarning: invalid v
  predictions[k].sum(axis=1)[:, np.newaxis])
```

```
n_estimators: 20, leaf_size: 10000
liblin: 0.9993, 1.0000,  0.9993, 0.6829
```

```
/usr/local/lib/python3.6/dist-packages/sklearn/ensemble/forest.py:453: UserWarning: Some inputs
  warn("Some inputs do not have OOB scores. "
/usr/local/lib/python3.6/dist-packages/sklearn/ensemble/forest.py:458: RuntimeWarning: invalid v
  predictions[k].sum(axis=1)[:, np.newaxis])
```

```
n_estimators: 25, leaf_size: 2
liblin: 1.0000, 1.0000,  1.0000, 0.8328
```

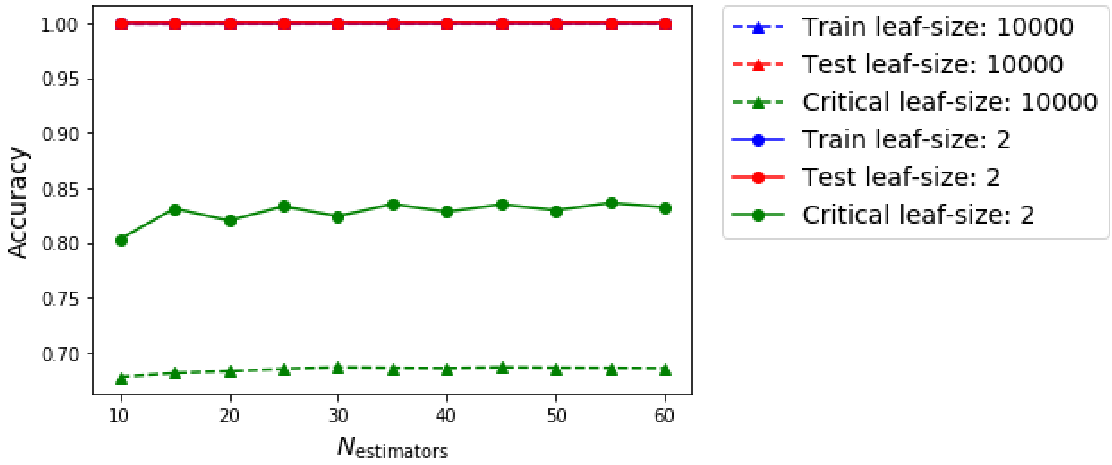
```
/usr/local/lib/python3.6/dist-packages/sklearn/ensemble/forest.py:453: UserWarning: Some inputs
  warn("Some inputs do not have OOB scores. "
/usr/local/lib/python3.6/dist-packages/sklearn/ensemble/forest.py:458: RuntimeWarning: invalid v
  predictions[k].sum(axis=1)[:, np.newaxis])
```

```
n_estimators: 25, leaf_size: 10000
liblin: 0.9993, 1.0000,  0.9993, 0.6848
```

```
n_estimators: 30, leaf_size: 2
liblin: 1.0000, 1.0000,  1.0000, 0.8238

n_estimators: 30, leaf_size: 10000
liblin: 0.9993, 1.0000,  0.9993, 0.6864

n_estimators: 35, leaf_size: 2
liblin: 1.0000, 1.0000,  1.0000, 0.8348

n_estimators: 35, leaf_size: 10000
liblin: 0.9993, 1.0000,  0.9993, 0.6857

n_estimators: 40, leaf_size: 2
liblin: 1.0000, 1.0000,  1.0000, 0.8279

n_estimators: 40, leaf_size: 10000
liblin: 0.9993, 1.0000,  0.9993, 0.6854

n_estimators: 45, leaf_size: 2
liblin: 1.0000, 1.0000,  1.0000, 0.8345

n_estimators: 45, leaf_size: 10000
liblin: 0.9993, 1.0000,  0.9993, 0.6864

n_estimators: 50, leaf_size: 2
liblin: 1.0000, 1.0000,  1.0000, 0.8292

n_estimators: 50, leaf_size: 10000
liblin: 0.9993, 1.0000,  0.9993, 0.6859

n_estimators: 55, leaf_size: 2
liblin: 1.0000, 1.0000,  1.0000, 0.8360

n_estimators: 55, leaf_size: 10000
liblin: 0.9993, 1.0000,  0.9993, 0.6857
```

```
n_estimators: 60, leaf_size: 2
liblin: 1.0000, 1.0000,  1.0000, 0.8319


n_estimators: 60, leaf_size: 10000
liblin: 0.9993, 1.0000,  0.9993, 0.6853
```

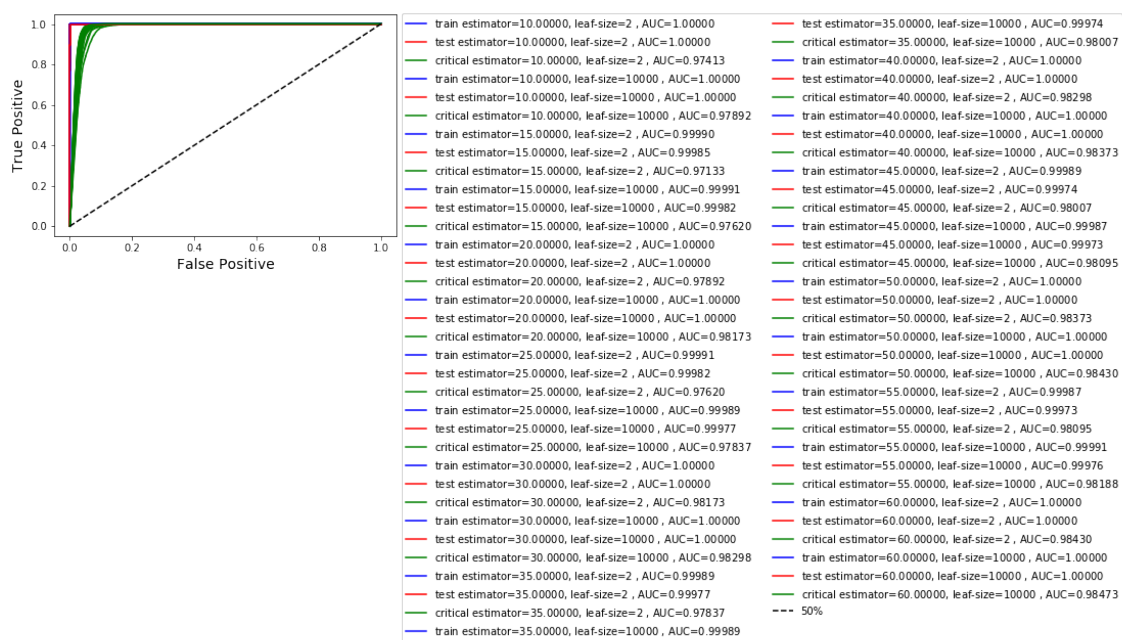
```
In [62]: plt.figure()
         plt.plot(n_estimators,RFC_train_accuracy[:,1],'--b^',label='Train leaf-size: 10000')
         plt.plot(n_estimators,RFC_test_accuracy[:,1],'--r^',label='Test leaf-size: 10000')
         plt.plot(n_estimators,RFC_critical_accuracy[:,1],'--g^',label='Critical leaf-size: 1000

         plt.plot(n_estimators,RFC_train_accuracy[:,0],'o-b',label='Train leaf-size: 2')
         plt.plot(n_estimators,RFC_test_accuracy[:,0],'o-r',label='Test leaf-size: 2')
         plt.plot(n_estimators,RFC_critical_accuracy[:,0],'o-g',label='Critical leaf-size: 2')

         plt.xlabel('$N_\mathrm{estimators}$', fontsize=14)
         plt.ylabel('Accuracy', fontsize=14)
         lgd=plt.legend(bbox_to_anchor=(1.05, 1), loc=2, borderaxespad=0., fontsize=14)

         plt.show()
```



Again we can plot an ROC-curve to see how well the prediction is.

```
In [66]: from sklearn.metrics import roc_curve, roc_auc_score
```

```python
rfc_preds = [rfc_train_preds, rfc_test_preds, rfc_critical_preds]
Ys = [Y_train, Y_test, Y_critical]
labs = ["train", "test", "critical"]
ttc_colors = ['blue', 'red', 'green']

for i,e in enumerate(n_estimators):
    for j,l in enumerate(leaf_sizes):
        for k,rp in enumerate(rfc_preds):
            rfc_tpr, rfc_fpr, _ = roc_curve(Ys[k], rp[i*m+j])

            rfc_auc = 1-roc_auc_score(Ys[k], rp[i+j*m])

            plt.plot(rfc_fpr, rfc_tpr, ttc_colors[k], label=labs[k] + \
                     " estimator=$%.5f$, leaf-size=$%.5g$ , AUC=$%.5f$"
                     % (e, l, rfc_auc))
        # end fork
    # end forj
# end fori

plt.plot((0,1), (0,1), "--k", label='50%')

plt.legend(bbox_to_anchor=(1.0, 1.027), fancybox=True, shadow=True, ncol=2)
plt.xlabel("False Positive", fontsize=14)
plt.ylabel("True Positive", fontsize=14)
plt.show()
```



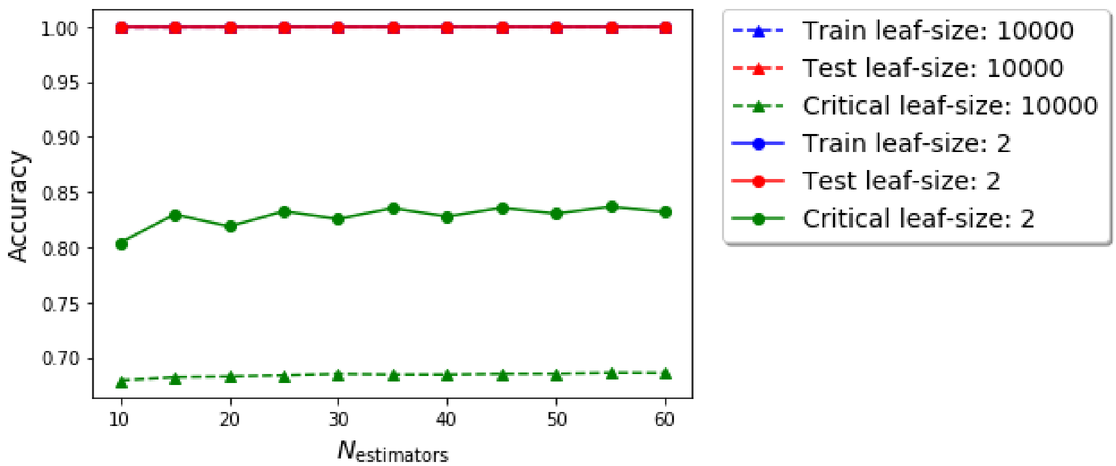
And secondly the Extremely Randomized Trees.

```
In [67]: from sklearn.ensemble import ExtraTreesClassifier

         ETC_train_accuracy=np.zeros((n,m))
         ETC_test_accuracy=np.zeros((n,m))
         ETC_critical_accuracy=np.zeros((n,m))

         etc_train_preds = []
         etc_test_preds = []
         etc_critical_preds = []

         print('train test critical')
         for i in range(0,n):
             for j in range(0,m):
                 ETC = ExtraTreesClassifier(n_estimators=n_estimators[i], max_depth=None,
                                            min_samples_split=leaf_sizes[j],random_state=0)
                 ETC.fit(X_train, Y_train)

                 ETC_train_accuracy[i,j] = ETC.score(X_train,Y_train)
                 ETC_test_accuracy[i,j] = ETC.score(X_test,Y_test)
                 ETC_critical_accuracy[i,j] = ETC.score(X_critical,Y_critical)

                 etc_train_preds.append(ETC.predict_proba(X_train)[:,0])
                 etc_test_preds.append(ETC.predict_proba(X_test)[:,0])
                 etc_critical_preds.append(ETC.predict_proba(X_critical)[:,0])

                 print('n_estimators: ' + str(n_estimators[i]) + ', leaf_size: ' + str(leaf_size
                 print('liblin: %0.4f,  %0.4f, %0.4f \n' % (ETC_train_accuracy[i,j],
                                                              ETC_test_accuracy[i,j],
                                                              ETC_critical_accuracy[i,j]))
```

```
train test critical
n_estimators: 10, leaf_size: 2
liblin: 1.0000,  1.0000, 0.8039

n_estimators: 10, leaf_size: 10000
liblin: 0.9991,  0.9991, 0.6789

n_estimators: 15, leaf_size: 2
liblin: 1.0000,  1.0000, 0.8297

n_estimators: 15, leaf_size: 10000
liblin: 0.9992,  0.9992, 0.6819

n_estimators: 20, leaf_size: 2
liblin: 1.0000,  1.0000, 0.8187

n_estimators: 20, leaf_size: 10000
liblin: 0.9993,  0.9992, 0.6825
```

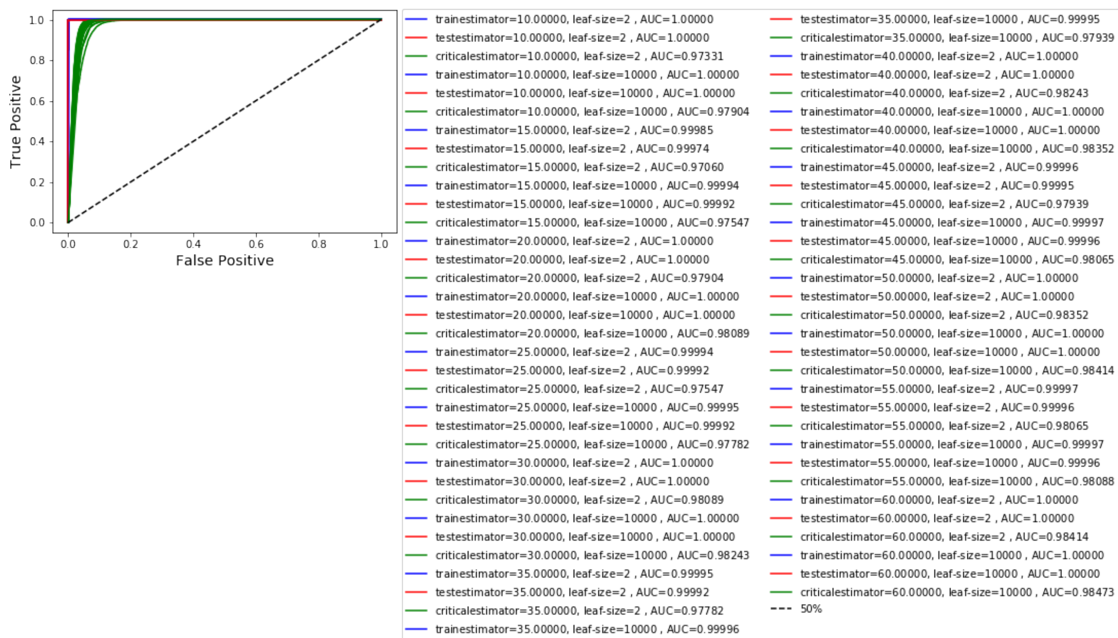
```
n_estimators: 25, leaf_size: 2
liblin: 1.0000,  1.0000, 0.8324

n_estimators: 25, leaf_size: 10000
liblin: 0.9993,  0.9992, 0.6835

n_estimators: 30, leaf_size: 2
liblin: 1.0000,  1.0000, 0.8255

n_estimators: 30, leaf_size: 10000
liblin: 0.9993,  0.9992, 0.6849

n_estimators: 35, leaf_size: 2
liblin: 1.0000,  1.0000, 0.8352

n_estimators: 35, leaf_size: 10000
liblin: 0.9993,  0.9992, 0.6843

n_estimators: 40, leaf_size: 2
liblin: 1.0000,  1.0000, 0.8276

n_estimators: 40, leaf_size: 10000
liblin: 0.9993,  0.9993, 0.6843

n_estimators: 45, leaf_size: 2
liblin: 1.0000,  1.0000, 0.8355

n_estimators: 45, leaf_size: 10000
liblin: 0.9993,  0.9993, 0.6850

n_estimators: 50, leaf_size: 2
liblin: 1.0000,  1.0000, 0.8303

n_estimators: 50, leaf_size: 10000
liblin: 0.9993,  0.9993, 0.6850

n_estimators: 55, leaf_size: 2
liblin: 1.0000,  1.0000, 0.8366

n_estimators: 55, leaf_size: 10000
liblin: 0.9993,  0.9993, 0.6859

n_estimators: 60, leaf_size: 2
liblin: 1.0000,  1.0000, 0.8317

n_estimators: 60, leaf_size: 10000
liblin: 0.9993,  0.9993, 0.6857
```

```
In [68]: # plot accuracy against regularisation strength
         plt.figure()
         plt.plot(n_estimators,ETC_train_accuracy[:,1],'--b^',label='Train leaf-size: 10000')
         plt.plot(n_estimators,ETC_test_accuracy[:,1],'--r^',label='Test leaf-size: 10000')
         plt.plot(n_estimators,ETC_critical_accuracy[:,1],'--g^',label='Critical leaf-size: 1000

         plt.plot(n_estimators,ETC_train_accuracy[:,0],'o-b',label='Train leaf-size: 2')
         plt.plot(n_estimators,ETC_test_accuracy[:,0],'o-r',label='Test leaf-size: 2')
         plt.plot(n_estimators,ETC_critical_accuracy[:,0],'o-g',label='Critical leaf-size: 2')

         plt.xlabel('$N_\mathrm{estimators}$', fontsize=14)
         plt.ylabel('Accuracy', fontsize=14)
         plt.legend(bbox_to_anchor=(1.05, 1), loc=2, borderaxespad=0., fancybox=True, shadow=Tru

         plt.show()
```




```
In [70]: from sklearn.metrics import roc_curve, roc_auc_score

         etc_preds = [etc_train_preds, etc_test_preds, etc_critical_preds]

         for i,e in enumerate(n_estimators):
             for j,l in enumerate(leaf_sizes):
                 for k,ep in enumerate(etc_preds):
                     etc_tpr, etc_fpr, _ = roc_curve(Ys[k], ep[i*m+j])

                     etc_auc = 1-roc_auc_score(Ys[k], ep[i+j*m])

                     plt.plot(etc_fpr, etc_tpr, ttc_colors[k], label=labs[k] + \
```

```
                          "estimator=$%.5f$, leaf-size=$%.5g$ , AUC=$%.5f$"
                          % (e, l, etc_auc))
        # end fok
    # end forj
# end fori

plt.plot((0,1), (0,1), "--k", label='50%')

plt.legend(bbox_to_anchor=(1.0, 1.027), fancybox=True, shadow=True, ncol=2)
plt.xlabel("False Positive", fontsize=14)
plt.ylabel("True Positive", fontsize=14)
plt.show()
```



As we can see with both the bagging and the randomized trees the performance is good. The critical case is still hard to determine, as is expected. In comparison to the logistic regression, the random forest seems to perform better

3.1.4 Classifying the Ising Model Phase Using Neural Networks

Just as we could use the logistic regression and random forest methods to find the phases of the Ising model we can use a feed-forward neural network to do the same. We will use the libraries TensorFlow and Keras. First let us make a class to load the data and to shuffle the data as the latter is useful in the training procedure in TensorFlow.

```
In [31]: import argparse
         import os
         import pickle
```

```
import collections
import numpy as np
from sklearn.model_selection import train_test_split
import tensorflow as tf
from tensorflow.python.framework import dtypes
from keras.utils import to_categorical

os.environ['TF_CPP_MIN_LOG_LEVEL'] = '2'

tf.set_random_seed(12)

class DataSet(object):
    def __init__(self, data_X, data_Y, dtype=dtypes.float32):
        dtype = dtypes.as_dtype(dtype).base_dtype
        if dtype not in (dtypes.uint8, dtypes.float32):
            raise TypeError('Invalid dtype %r, expected uint8 or float32' % dtype)

        assert data_X.shape[0] == data_Y.shape[0], ('data_X.shape: %s data_Y.shape: %s'

        self.num_examples = data_X.shape[0]

        if dtype == dtypes.float32:
            data_X = data_X.astype(np.float32)
        # end if

        self.data_X = data_X
        self.data_Y = data_Y

        self.epochs_completed = 0
        self.index_in_epoch = 0
    # end __init__

    def next_batch(self, batch_size, seed=None):
        """Return the next `batch_size` examples from this data set."""

        if seed:
            np.random.seed(seed)
        # end if

        start = self.index_in_epoch
        self.index_in_epoch += batch_size
        if self.index_in_epoch > self.num_examples:
            # Finished epoch
            self.epochs_completed += 1

            # Shuffle the data
            perm = np.arange(self.num_examples)
            np.random.shuffle(perm)
```

```
                self.data_X = self.data_X[perm]
                self.data_Y = self.data_Y[perm]

                # Start next epoch
                start = 0
                self.index_in_epoch = batch_size
                assert batch_size <= self.num_examples
            # end if

            end = self.index_in_epoch

            return self.data_X[start:end], self.data_Y[start:end]
        # end function next_batch
    # end class DataSet

    def read_data_set(dtype=dtypes.float32, train_size=80000, validation_size=5000):
        """read and reshape data"""

        # load data (all of it)
        data_path = "IsingData/"
        data = pickle.load(open(data_path + "Ising2DFM_reSample_L40_T=All.pkl", 'rb'))
        data = np.unpackbits(data).reshape(-1, 1600)
        data = data.astype('int')
        data[np.where(data==0)] = -1

        # load labels (all of it)
        labels = pickle.load(open(data_path + "Ising2DFM_reSample_L40_T=All_labels.pkl", "r

        # divide data into ordered, critical and disordered
        X_ordered=data[:70000,:]
        Y_ordered=labels[:70000]

        X_critical=data[70000:100000,:]
        Y_critical=labels[70000:100000]

        X_disordered=data[100000:,:]
        Y_disordered=labels[100000:]

        del data,labels

        # define training and test
        X=np.concatenate((X_ordered,X_disordered))
        Y=np.concatenate((Y_ordered,Y_disordered))

        del X_ordered, X_disordered, Y_ordered, Y_disordered

        X_train, X_test, Y_train, Y_test = train_test_split(X, Y, train_size=train_size)
```

```
            del X,Y

            # make data categorical
            Y_train = to_categorical(Y_train)
            Y_test = to_categorical(Y_test)
            Y_critical = to_categorical(Y_critical)

            X_validation = X_train[:validation_size]
            Y_validation = Y_train[:validation_size]
            X_train = X_train[validation_size:]
            Y_train = Y_train[validation_size:]

            # create data sets
            train = DataSet(X_train, Y_train, dtype=dtype)
            validation = DataSet(X_validation, Y_validation, dtype=dtype)
            test = DataSet(X_test, Y_test, dtype=dtype)
            critical = DataSet(X_critical, Y_critical, dtype=dtype)

            Datasets = collections.namedtuple('Datasets', ['train', 'validation', 'test', 'crit

            return Datasets(train=train, validation=validation, test=test, critical=critical)
```

```
/usr/lib/python3/dist-packages/h5py/__init__.py:36: FutureWarning: Conversion of the second argu
  from ._conv import register_converters as _register_converters
Using TensorFlow backend.
```

With the function for handling the data available we can proceed with creating the neural net and its architecture. We will make the DNN with a class model with some placeholders used by TensorFlow.

```
In [32]: class model(object):
             def __init__(self, N_neurons, opt_kwargs):
                 self.global_step = tf.Variable(0, dtype=tf.int32, trainable=False, name='global

                 self.L = 40
                 self.n_feats = self.L**2
                 self.n_categories = 2

                 self.create_placeholders()
                 self.deep_layer_neurons = N_neurons
                 self.create_DNN()
                 self.create_loss()
                 self.create_optimiser(opt_kwargs)
                 self.create_accuracy()
             # end __init__

             def create_placeholders(self):
```

```
    """define placeholders used by TensorFlow"""
    with tf.name_scope('data'):
        self.X = tf.placeholder(tf.float32, shape=(None, self.n_feats), name="X_dat
        self.Y = tf.placeholder(tf.float32, shape=(None, self.n_categories), name="
        self.dropout_keepprob = tf.placeholder(tf.float32, name="keep_probability")
    # end with
# end function create_placeholders

def _weight_variable(self, shape, name='', dtype=tf.float32):
    """make a weight of given shape"""
    initial = tf.truncated_normal(shape, stddev=0.1)
    return tf.Variable(initial, dtype=dtype, name=name)
# end function _weight_variable

def _bias_variable(self, shape, name='', dtype=tf.float32):
    """create bias variable of given shape"""
    initial = tf.constant(0,1, shape=shape)
    return tf.Variable(initial, dtype=dtype, name=name)
# end function _bias_variable

def create_DNN(self):
    """create layers"""
    with tf.name_scope('DNN'):
        W_fc1 = self._weight_variable([self.n_feats, self.deep_layer_neurons], name
                                      dtype=tf.float32)
        b_fc1 = self._bias_variable([self.deep_layer_neurons], name='fc1', dtype=tf

        a_fc1 = tf.nn.relu(tf.matmul(self.X, W_fc1) + b_fc1)

        W_fc2 = self._weight_variable([self.deep_layer_neurons, self.n_categories],
                                      dtype=tf.float32)
        b_fc2 = self._bias_variable([self.n_categories], name='fc2', dtype=tf.float

        self.Y_predicted = tf.matmul(a_fc1, W_fc2) + b_fc2
    # end with
# end function create_DNN

def create_loss(self):
    with tf.name_scope('loss'):
        self.loss = tf.reduce_mean(tf.nn.softmax_cross_entropy_with_logits_v2(label
                                                                             logit
    # end with
# end function create_loss

def create_optimiser(self, opt_kwarg):
    with tf.name_scope('optimiser'):
        self.optimizer = tf.train.GradientDescentOptimizer(**opt_kwarg).minimize(se
                                                                           global_s
```

```
            # end with
        # end function crate_optimiser

        def create_accuracy(self):
            with tf.name_scope('accuracy'):
                correct_prediction = tf.equal(tf.argmax(self.Y, 1), tf.argmax(self.Y_predic
                correct_prediction = tf.cast(correct_prediction, tf.float64)
                self.accuracy = tf.reduce_mean(correct_prediction)
            # end with
        # end function create_accuracy
    # end class model
```

The next part is to train the model and evaluate the performance.

```
In [33]: def evaluate_model(neurons, lr, Ising_Data, verbose):
             training_epochs = 100
             batch_size = 100

             # SGD parameters
             opt_params = dict(learning_rate=lr)

             # create DNN
             DNN = model(neurons, opt_params)

             with tf.Session() as sess:
                 sess.run(tf.global_variables_initializer())

                 # train DNN
                 for epoch in range(training_epochs):
                     batch_X, batch_Y = Ising_Data.train.next_batch(batch_size)

                     loss_batch, _ = sess.run([DNN.loss, DNN.optimizer],
                                             feed_dict={DNN.X: batch_X,
                                                        DNN.Y: batch_Y,
                                                        DNN.dropout_keepprob: 0.5})
                     accuracy = sess.run(DNN.accuracy,
                                         feed_dict={DNN.X: Ising_Data.train.data_X,
                                                    DNN.Y: Ising_Data.train.data_Y,
                                                    DNN.dropout_keepprob: 0.5})
                     step = sess.run(DNN.global_step)
                 # end for epoch

                 # test DNN performance on entire train, test and critical data sets
                 train_loss, train_accuracy = sess.run([DNN.loss, DNN.accuracy],
                                                       feed_dict={DNN.X: Ising_Data.train.data_X
                                                                  DNN.Y: Ising_Data.train.data_Y
                                                                  DNN.dropout_keepprob: 0.5})
```

```
            test_loss, test_accuracy = sess.run([DNN.loss, DNN.accuracy],
                                        feed_dict={DNN.X: Ising_Data.test.data_X,
                                                   DNN.Y: Ising_Data.test.data_Y,
                                                   DNN.dropout_keepprob: 1.0})

            critical_loss, critical_accuracy = sess.run([DNN.loss, DNN.accuracy],
                                                feed_dict={DNN.X: Ising_Data.critic
                                                           DNN.Y: Ising_Data.critic
                                                           DNN.dropout_keepprob: 1.

            return train_loss, train_accuracy, test_loss, test_accuracy, critical_loss, cri
        # end with
    # end function evaluate_model
```

Finally in order to study the DNN fully we need to account for the hyperparameters, these are the hidden layers and different SGD learning rates. This is done by a grid search over a grid with said hyperparameters.

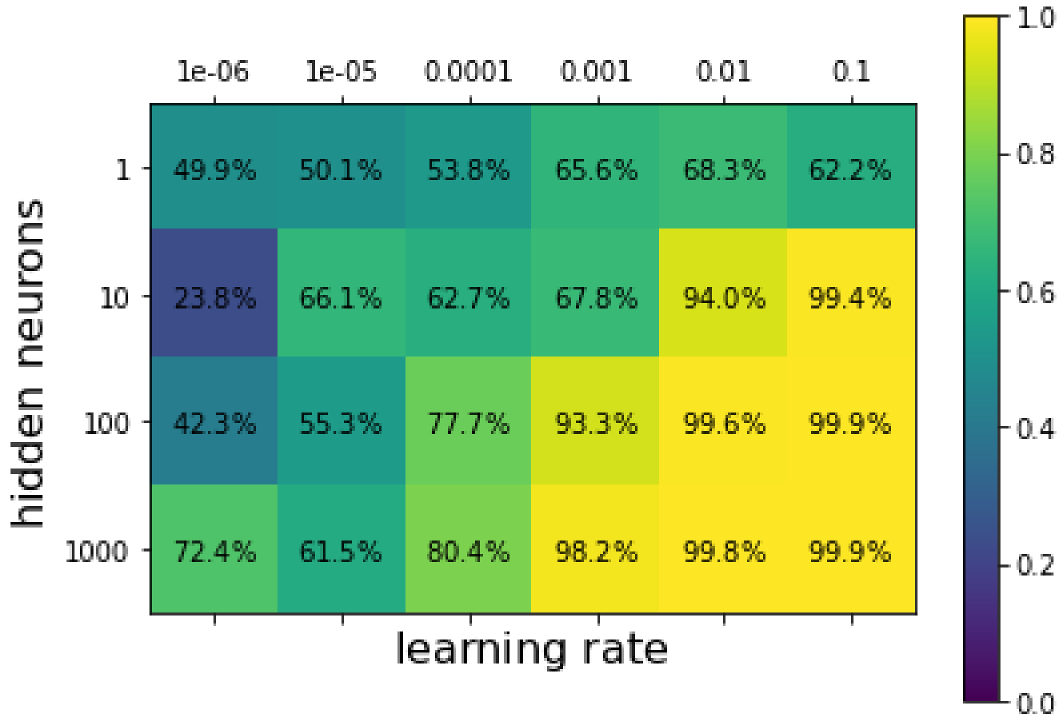
```
In [35]: import matplotlib.pyplot as plt
         def grid_search(verbose):
             """perform grid_search over different learning rates and number of hidden layer neu

             # load data
             Ising_Data = read_data_set()

             N_neurons = np.logspace(0,3,4).astype(np.int32)
             learning_rates = np.logspace(-6,-1,6)

             train_loss=np.zeros((len(N_neurons),len(learning_rates)),dtype=np.float64)
             train_accuracy=np.zeros_like(train_loss)
             test_loss=np.zeros_like(train_loss)
             test_accuracy=np.zeros_like(train_loss)
             critical_loss=np.zeros_like(train_loss)
             critical_accuracy=np.zeros_like(train_loss)

             # do grid search
             for i, neurons in enumerate(N_neurons):
                 for j, lr in enumerate(learning_rates):

                     print("training DNN with %4d neurons and SGD lr=%0.6f." %(neurons,lr) )

                     train_loss[i,j],train_accuracy[i,j],\
                     test_loss[i,j],test_accuracy[i,j],\
                     critical_loss[i,j],critical_accuracy[i,j] = evaluate_model(neurons,lr,Ising


             plot_DNNdata(learning_rates,N_neurons,train_accuracy)
```

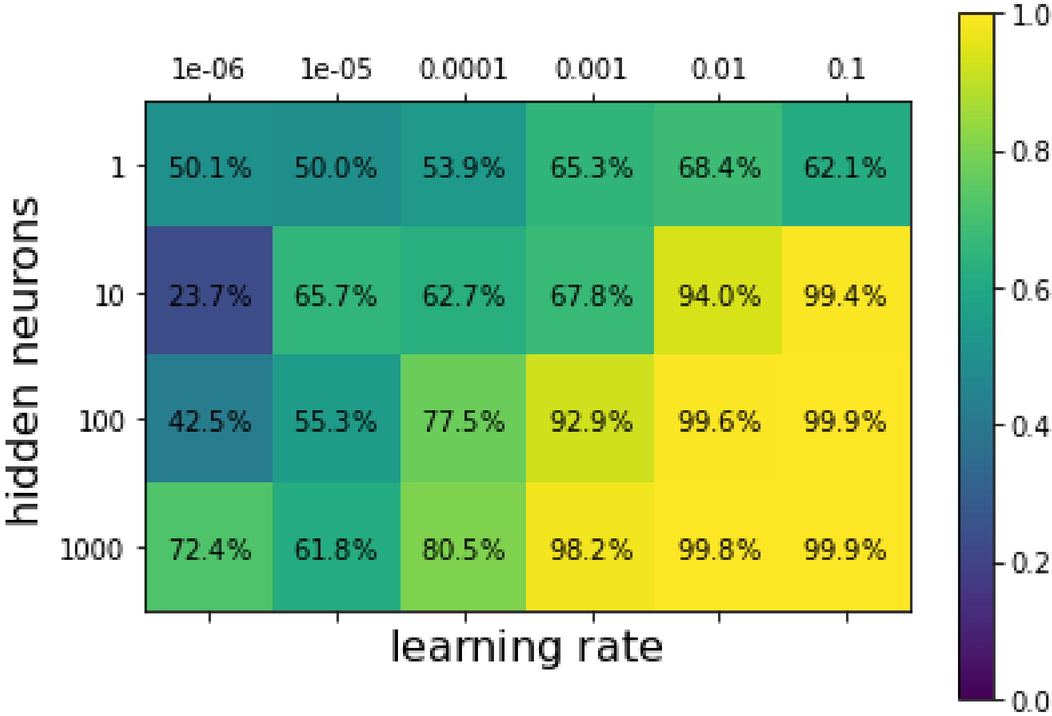
```
        plot_DNNdata(learning_rates,N_neurons,test_accuracy)
        plot_DNNdata(learning_rates,N_neurons,critical_accuracy)
    # end function grid_search

    def plot_DNNdata(x,y,data):

        # plot results
        fontsize=16

        fig = plt.figure()
        ax = fig.add_subplot(111)
        cax = ax.matshow(data, interpolation='nearest', vmin=0, vmax=1)
        fig.colorbar(cax)

        # put text on matrix elements
        for i, x_val in enumerate(np.arange(len(x))):
            for j, y_val in enumerate(np.arange(len(y))):
                c = "${0:.1f}\\%$".format( 100*data[j,i])
                ax.text(x_val, y_val, c, va='center', ha='center')

        # convert axis vaues to to string labels
        x=[str(i) for i in x]
        y=[str(i) for i in y]


        ax.set_xticklabels(['']+x)
        ax.set_yticklabels(['']+y)

        ax.set_xlabel('$\\mathrm{learning\\ rate}$',fontsize=fontsize)
        ax.set_ylabel('$\\mathrm{hidden\\ neurons}$',fontsize=fontsize)

        plt.tight_layout()

        plt.show()
```

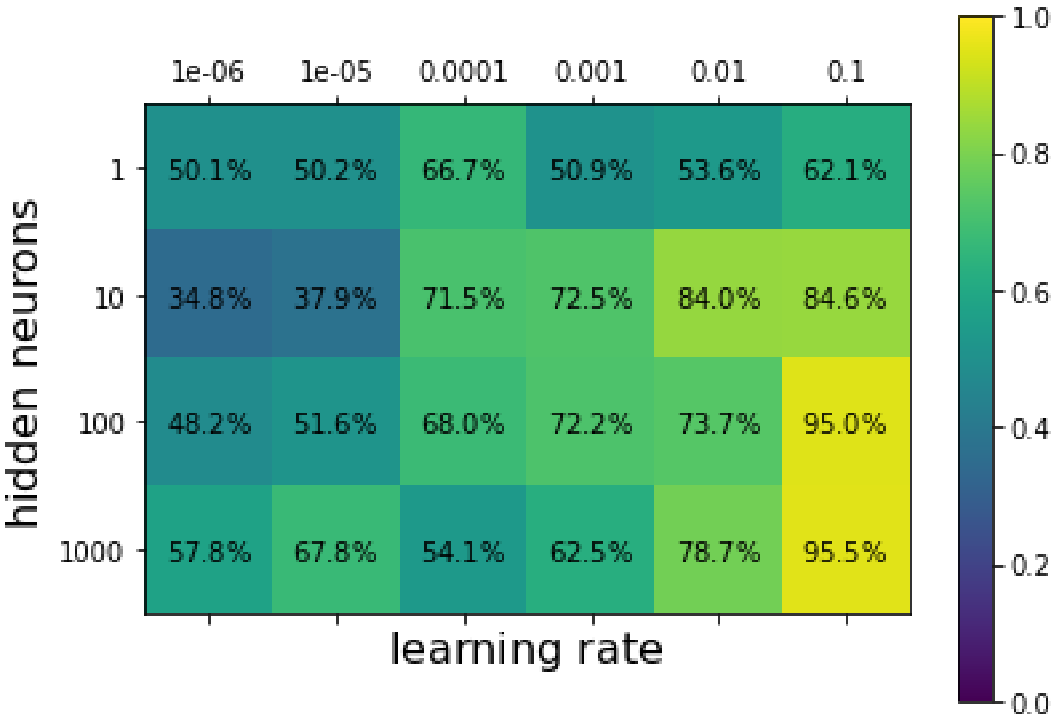
```
In [36]: grid_search(False)
```

```
/usr/local/lib/python3.6/dist-packages/sklearn/model_selection/_split.py:2026: FutureWarning: Fr
  FutureWarning)


training DNN with    1 neurons and SGD lr=0.000001.
training DNN with    1 neurons and SGD lr=0.000010.
training DNN with    1 neurons and SGD lr=0.000100.
training DNN with    1 neurons and SGD lr=0.001000.
training DNN with    1 neurons and SGD lr=0.010000.
training DNN with    1 neurons and SGD lr=0.100000.
training DNN with   10 neurons and SGD lr=0.000001.
```

```
training DNN with   10 neurons and SGD lr=0.000010.
training DNN with   10 neurons and SGD lr=0.000100.
training DNN with   10 neurons and SGD lr=0.001000.
training DNN with   10 neurons and SGD lr=0.010000.
training DNN with   10 neurons and SGD lr=0.100000.
training DNN with  100 neurons and SGD lr=0.000001.
training DNN with  100 neurons and SGD lr=0.000010.
training DNN with  100 neurons and SGD lr=0.000100.
training DNN with  100 neurons and SGD lr=0.001000.
training DNN with  100 neurons and SGD lr=0.010000.
training DNN with  100 neurons and SGD lr=0.100000.
training DNN with 1000 neurons and SGD lr=0.000001.
training DNN with 1000 neurons and SGD lr=0.000010.
training DNN with 1000 neurons and SGD lr=0.000100.
training DNN with 1000 neurons and SGD lr=0.001000.
training DNN with 1000 neurons and SGD lr=0.010000.
training DNN with 1000 neurons and SGD lr=0.100000.
```




1e-06
1e-05
0.0001
0.001
0.01
0.1
1
10
100
1000
hidden neurons
learning rate
50.1% 50.0% 53.9% 65.3% 68.4% 62.1%
23.7% 65.7% 62.7% 67.8% 94.0% 99.4%
42.5% 55.3% 77.5% 92.9% 99.6% 99.9%
72.4% 61.8% 80.5% 98.2% 99.8% 99.9%
1.0
0.8
0.6
0.4
0.2
0.0


1e-06
1e-05
0.0001
0.001
0.01
0.1
1
10
100
1000
hidden neurons
learning rate
50.1% 50.2% 66.7% 50.9% 53.6% 62.1%
34.8% 37.9% 71.5% 72.5% 84.0% 84.6%
48.2% 51.6% 68.0% 72.2% 73.7% 95.0%
57.8% 67.8% 54.1% 62.5% 78.7% 95.5%
1.0
0.8
0.6
0.4
0.2
0.0