MI - H5

December 1, 2016

In [2]:
```
import numpy as np
import matplotlib.pyplot as plt
import matplotlib.cm as cm
import mpl_toolkits.mplot3d
import mpl_toolkits.axes_grid1 as plt_ax
import itertools
%matplotlib inline

def plot(ax, data, enum=False, title='', labels=None, legend=False, **kwarg
    plotted = None
    if enum:
        plotted = ax.plot(data)
    else:
        mapping = np.array(data).T
        plotted = ax.plot(mapping[0], mapping[1], **kwargs)
    if labels:
        ax.set_xlabel(labels[0])
        if (len(labels) > 1):
            ax.set_ylabel(labels[1])
    if legend:
        ax.legend(bbox_to_anchor=(1.05, 1), loc=2, borderaxespad=0)
    ax.set_title(title)
    ax.grid(True)
    return plotted

def scatter(ax, data, enum=False, title='', labels=None, legend=False, **kw
    scattered = None
    if enum:
        scattered = ax.scatter(range(len(data)), data, **kwargs)
    else:
        mapping = np.array(data).T
        scattered = ax.scatter(mapping[0], mapping[1], **kwargs)
    if labels:
        ax.set_xlabel(labels[0])
        if (len(labels) > 1):
            ax.set_ylabel(labels[1])
    if legend:
        ax.legend(bbox_to_anchor=(1.05, 1), loc=2, borderaxespad=0)
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    ax.set_title(title)
    ax.grid(True)
    ax.scatter(*np.mean(data, axis=0), color='red', s=40)
    return scattered

def plot_ridge(ridge):
    fig = plt.figure(figsize=(12, 3))
    ax1 = fig.add_subplot(131, projection='3d')
    ax1.scatter(*ridge.T)
    ax1.set_xticks(ax1.get_xticks()[::2])
    ax1.set_yticks(ax1.get_yticks()[::2])
    ax1.set_zticks(ax1.get_zticks()[::2])
    ax1.set_xlabel('x1')
    ax1.set_ylabel('x2')
    ax1.set_zlabel('y')
    ax1.scatter(*ridge.mean(axis=0), color='red', s=70)
    ax2 = fig.add_subplot(132)
    scatter(ax2, ridge[:, [0, 2]], labels=['x1', 'y'])
    ax2.set_xticks(ax2.get_xticks()[::2])
    ax3 = fig.add_subplot(133)
    scatter(ax3, ridge[:, [1, 2]], labels=['x2', 'y'])
    fig.tight_layout()

def scatter_set(data1, data2, titles=['Training set', 'Validation set']):
    min_ = min(np.concatenate([data1[:, 2], data2[:, 2]]))
    max_ = max(np.concatenate([data1[:, 2], data2[:, 2]]))
    fig, axes = plt.subplots(1, 2, figsize=(13, 4))
    for data, ax, title in zip([data1, data2], axes, titles):
        dataX = data[:, :2]
        dataY = data[:, 2]
        C = dataX.T.dot(dataX) / dataX.shape[0]
        _, ev = np.linalg.eigh(C)
        scatter_ax = scatter(ax, dataX, c=dataY, vmin=min_, vmax=max_, s=np
        ax.arrow(0, 0, *ev[0], head_width=0.2, head_length=0.1, fc='k', ec=
        ax.arrow(0, 0, *ev[1], head_width=0.2, head_length=0.1, fc='k', ec=
    fig.subplots_adjust(right=0.85)
    fig.colorbar(scatter_ax, cmap='jet', cax=fig.add_axes([0.9, 0.15, 0.03,

def plot_heatmaps(monomials):
    powers = np.array([[0, 0], [1, 0], [0, 1], [2, 0], [1, 1], [0, 2], [3,
    fig, axes = plt.subplots(5, 2, figsize=(10, 16))
    for row, axesRow in enumerate(axes):
        for col, ax in enumerate(axesRow):
            i = row * 2 + col
            max_ = 5  # monomials[i, :10].max()
            img = ax.imshow(monomials[i, :10].T, extent=[-40, 40, -35, 35],
            cax = plt_ax.make_axes_locatable(ax).append_axes("right", size=
            cbar = plt.colorbar(img, cax=cax)
```

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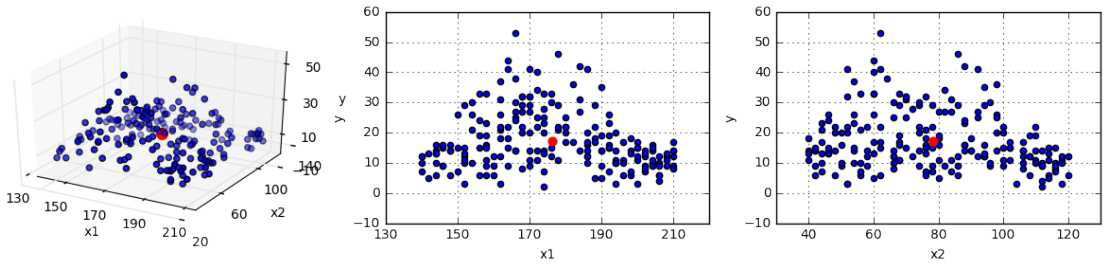
                ax.set_title(r'$degree = {}, \phi_{} = x_1^{} x_2^{}$'.format(p
                ax.set_ylabel('x1')
                ax.set_xlabel('x2')
            fig.subplots_adjust(hspace=.4, wspace=.3)

        def plot_mse(MSE, lambda_index='T'):
            fig, ax = plt.subplots(1, 1, figsize=(13, 4))
            meanlineprops = dict(linestyle='--', linewidth=2.5, color='green')
            ax.boxplot(MSE.T, meanprops=meanlineprops, meanline=True, showmeans=Tru
            ax.set_yscale('log')
            means = MSE.T.mean(axis=0)
            best_mse_index = np.argmin(means)
            ax.set_title(r'Boxplots for each lambda  -  $avg_{{min}} = {:.2f}$ at $
                means[best_mse_index], lambda_index, np.linspace(-4, 4, 81)[best_ms
            ax.grid(True)
            ax.set_xticks(ax.get_xticks()[::10])
            ax.set_xticklabels([r'$10^{{{}}}$'.format(x) for x in range(-4, 5)])
```

In [3]:
```
# Array of 200 observations {x_n, y_n} with x_n = [x_n_1, x_n_2]
training_ridge = np.loadtxt('TrainingRidge.csv', skiprows=1, dtype=bytes, c
plot_ridge(training_ridge)
# Array of 1476 combinations for [x_n_1, x_n_2] (36 x 41 grid) in same form
validation_ridge = np.loadtxt('ValidationRidge-Y.csv', skiprows=1, dtype=by
# data2 = Matrix(np.cov([[S(x1), S(x2), S(y)] for x1, x2, y in (training_ri
```

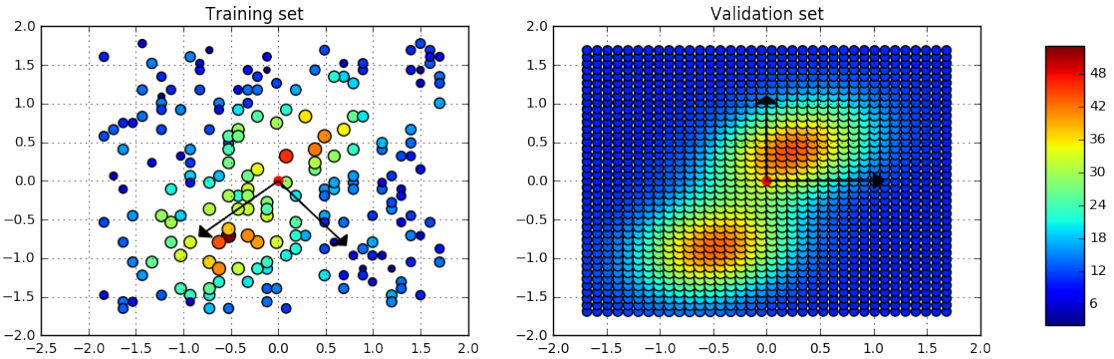


In [4]:
```
# Exercise 2 (a)
def whiten_data(ridge):
    ridge = np.copy(ridge)
    data = ridge[:, :2]
    # Centering
    data -= data.mean(axis=0)
    C = data.T.dot(data) / data.shape[0]
    w, V = np.linalg.eigh(C)
    L = np.diag(np.nan_to_num(1 / np.sqrt(w)))
    # Decorrelation
    data = V.T.dot(data.T).T
    # Whitening
```

```
        data = L.dot(V.T).dot(data.T).T
        ridge[:, :2] = data
        return ridge

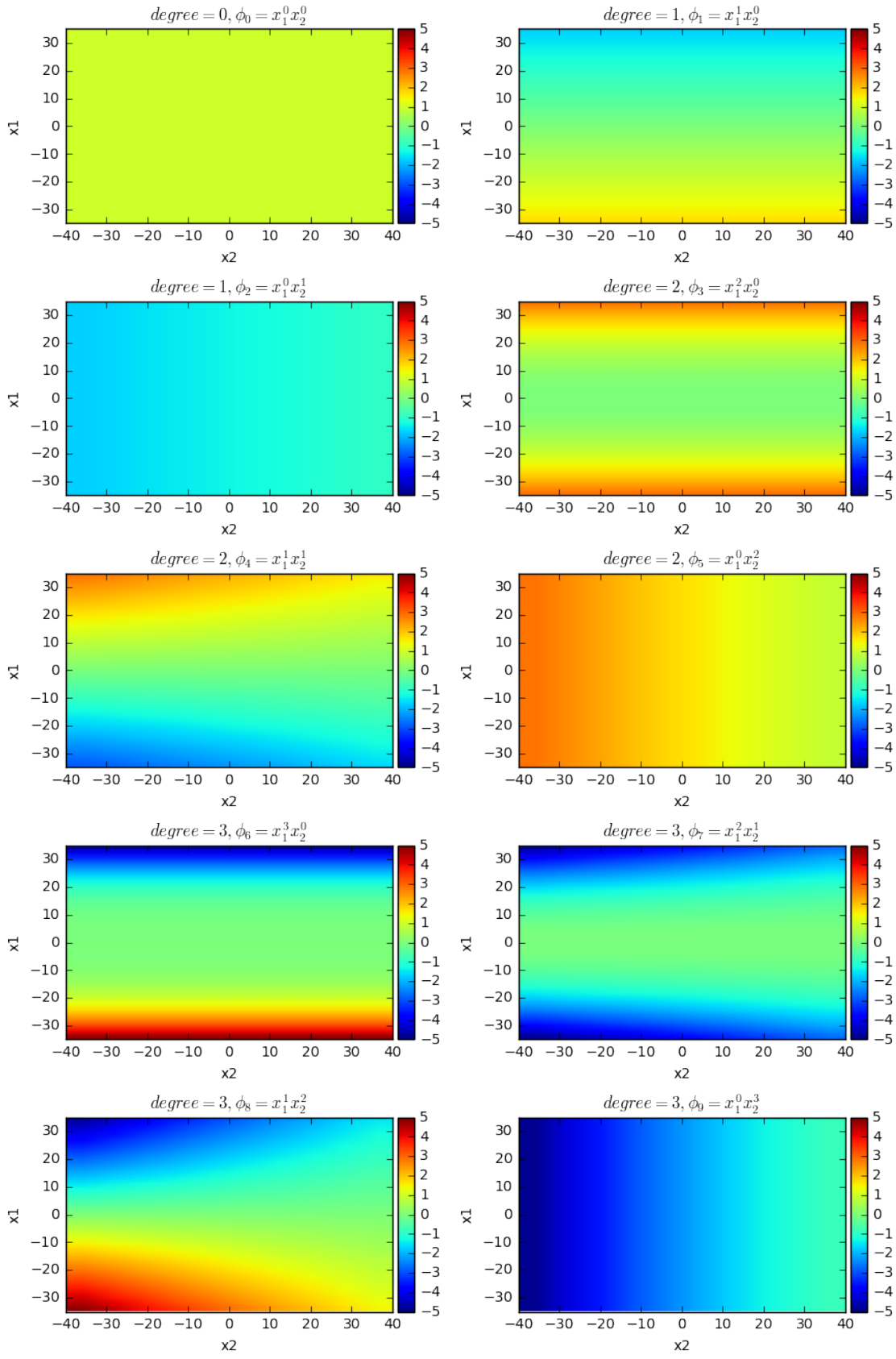
    training_whiten = whiten_data(training_ridge)
    validation_whiten = whiten_data(validation_ridge)
    scatter_set(training_whiten, validation_whiten)

    #FIXME: Training & validation set should look rotated (decorrelation missi
```



In [5]:
```
# Exercise 5.2 (b)
def monomial_matrix(ridge):
    def monomials(x1, x2, max_degree):
        for degree in range(max_degree + 1):
            for i in range(degree + 1):
                yield x1**(degree - i) * x2**i
    matrix = np.array([[x1, x2, monomials(x1, x2, 9), y] for x1, x2, y in r
    matrix = np.array([list(x) for x in matrix[:, 2]])
    return matrix

validation_monomial = monomial_matrix(validation_whiten)
training_monomial = monomial_matrix(training_whiten).T
plot_heatmaps(validation_monomial.T.reshape(55, 41, 36))
```

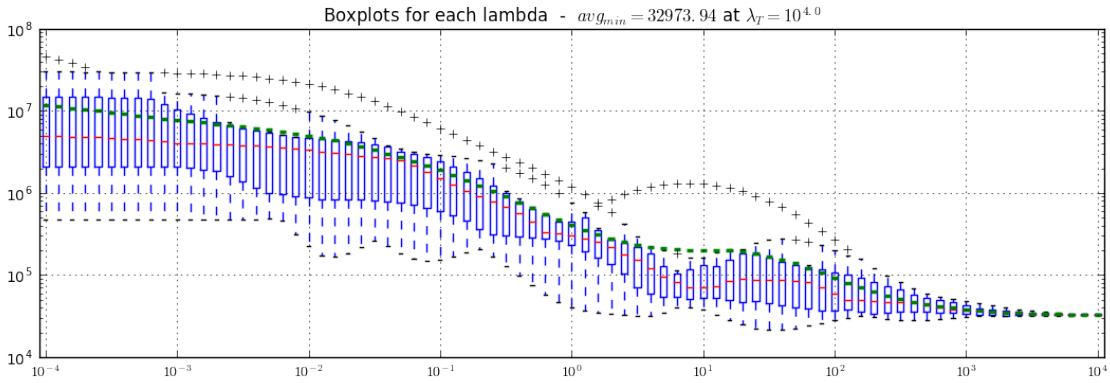

$degree = 0, \phi_0 = x_1^0 x_2^0$
$degree = 1, \phi_1 = x_1^1 x_2^0$
$degree = 1, \phi_2 = x_1^0 x_2^1$
$degree = 2, \phi_3 = x_1^2 x_2^0$
$degree = 2, \phi_4 = x_1^1 x_2^1$
$degree = 2, \phi_5 = x_1^0 x_2^2$
$degree = 3, \phi_6 = x_1^3 x_2^0$
$degree = 3, \phi_7 = x_1^2 x_2^1$
$degree = 3, \phi_8 = x_1^1 x_2^2$
$degree = 3, \phi_9 = x_1^0 x_2^3$
x1
x2

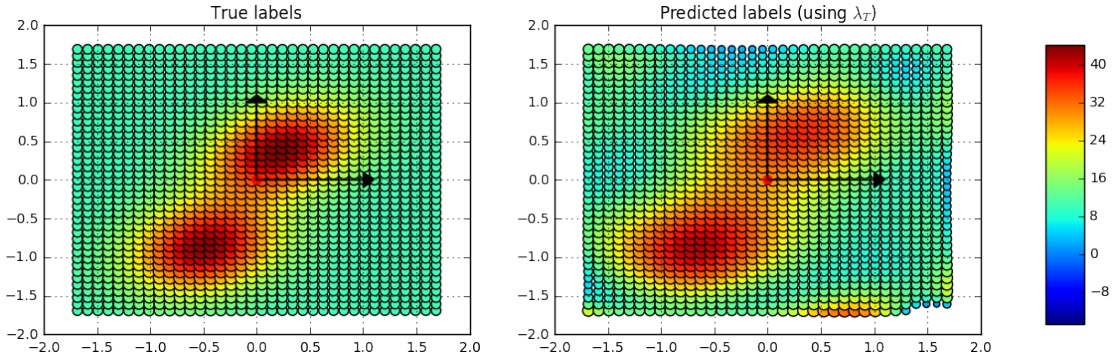
In [9]:
```
# Exercise 2 (c)
def weight_prediction(X, Y, lambda_):
    # Prediction function for the weight matrix using a weight decay term
    w = np.linalg.inv(X.dot(X.T) + lambda_ * np.identity(X.shape[0])).dot(X
    YT = w.T.dot(X)
    return YT, w

lambdas = 10**np.linspace(-4, 4, 81)
foldSize = 20
# 10-fold cross validation with training set (training_whiten) over all lam
MSE = np.zeros((len(lambdas), 10))
for j, lambda_ in enumerate(lambdas):
    for i in range(10):
        train_X = training_monomial[:, foldSize*i:foldSize*(i+1)]  # (55 x
        train_Y = training_ridge[foldSize*i:foldSize*(i+1), 2]  # (20 x 1)
        test_X = np.concatenate([
            training_monomial[:, :foldSize*i].T,
            training_monomial[:, foldSize*(i+1):].T,
        ]).T  # (55 x 180)
        test_Y = np.concatenate([
            training_ridge[:foldSize*i, 2],
            training_ridge[foldSize*(i+1):, 2],
        ])  # (180 x 1)
        # Regularization with weight-decay term
        _, w = weight_prediction(train_X, train_Y, lambda_)
        # Quadratic error function
        diff = w.T.dot(test_X) - test_Y
        MSE[j, i] = 0.5 * diff.dot(diff.T)
plot_mse(MSE)

# Compare predicted labels (using learned lambda) with true labels
lambdaT = lambdas[np.argmin(MSE.T.mean(axis=0))]
# FIXME: global minimum should be at 10^-1 (a bit shifted to the left), the
lambdaT = 10**(-1.2)
_, w = weight_prediction(training_monomial, training_ridge[:, 2], lambdaT)
YT = w.T.dot(validation_monomial.T)
prediction_set = np.array([(*x[:2], y) for x, y in zip(validation_whiten, Y
scatter_set(validation_whiten, prediction_set, titles=['True labels', r'Pre
```

```
c:\python\python35\lib\site-packages\ipykernel\__main__.py:71: RuntimeWarning: inva
```






```
In [ ]: # Exercise 2 (e)
        # Lerne lambda mit validation_set und plot wieder alles wie in 2c

        # 10-fold cross validation with training set (training_whiten) over all lam
        foldSize = 147
        MSE = np.zeros((len(lambdas), 10))
        for j, lambda_ in enumerate(lambdas):
            for i in range(10):
                train_X = validation_monomial[foldSize*i:foldSize*(i+1)].T  # (55 x
                train_Y = validation_ridge[foldSize*i:foldSize*(i+1), 2]  # (147 x
                test_X = np.concatenate([
                    validation_monomial[:foldSize*i],
                    validation_monomial[foldSize*(i+1):],
                ]).T
                test_Y = np.concatenate([
                    validation_ridge[:foldSize*i, 2],
                    validation_ridge[foldSize*(i+1):, 2],
                ])
                # Regularization with weight-decay term
```

```
            YT, w = weight_prediction(train_X, train_Y, lambda_)
            # Quadratic error function
            diff = w.T.dot(test_X) - test_Y
            MSE[j, i] = 0.5 * diff.dot(diff.T)
plot_mse(MSE, 'G')

# Compare predicted labels (using learned lambda) with true labels
lambdaG = lambdas[np.argmin(MSE.T.mean(axis=0))]
lambdaG = 0.05  # FIXME: Error in calculation for boxplot
best_YT, _ = weight_prediction(
    validation_monomial.T,
    validation_ridge[:, 2],
    lambdaG)
prediction_set = np.array([(*x[:2], y) for x, y in zip(validation_whiten, b
scatter_set(validation_whiten, prediction_set, titles=['True labels', r'Pre
```