Regularized Linear Regression with scikit-learn

Earlier we covered Ordinary Least Squares regression. In this posting we will build upon this foundation and introduce an important extension to linear regression, regularization (http://en.wikipedia.org/wiki/Regularization_(mathematics)), that makes it applicable for ill-posed problems (http://en.wikipedia.org/wiki/Ill-posed_problem) (e.g. number of predictors >> number of samples) and helps to prevent overfitting (http://en.wikipedia.org/wiki/Overfitting).

This is part of a series of blog posts showing how to do common statistical learning techniques with Python. We provide only a small amount of background on the concepts and techniques we cover, so if you'd like a more thorough explanation check out Introduction to Statistical Learning (http://www-bcf.usc.edu/~gareth/ISL/) or sign up for the free online course (http://online.stanford.edu/course/statistical-learning-winter-2014) run by the book's authors here.

Regularized Linear Regression

In a previous posting (http://www.datarobot.com/blog/multiple-regression-using-statsmodels/) we introduced linear regression and polynomial regression. Polynomial regression (http://en.wikipedia.org/wiki/Polynomial_regression) fits a n-th order polynomial to our data using least squares. There's a question that we didn't answer: which order of the polynomial should we choose? Clearly, the higher the order of the polynomial, the higher the complexity of the model. This is true both computationally and conceptually because in both cases we now have a higher number of adaptable parameters. The higher the complexity of a model the more variance it can capture. Given that computation is cheap, should we always pick the most complex model? As we will show below, the answer to this question is no: we have to strike a balance between variance and (inductive) bias: our model needs to have sufficient complexity to model the relationship between the predictors and the response, but it must not fit the idiosyncrasies of our training data, idiosyncrasies which will limit its ability to generalize to new, unseen cases.

This is best illustrated using a simple curve fitting example, which is adopted from C. Bishop's *Pattern Recognition and Machine Learning* (2007). Let's create a synthetic dataset by adding some random gaussian noise to a sinusoidal function.

In [1]:

```
%pylab inline

import numpy as np
from sklearn.linear_model import LinearRegression
from sklearn.linear_model import Ridge

from sklearn.cross_validation import train_test_split

try:
    from sklearn.preprocessing import PolynomialFeatures
    from sklearn.pipeline import make_pipeline
except ImportError:
    # use backports for sklearn 1.4
    # available from https://s3.amazonaws.com/datarobotblog/notebooks/sklearn_back
ports.py
    from sklearn_backports import PolynomialFeatures
    from sklearn_backports import make_pipeline

# ignore DeprecateWarnings by sklearn
import warnings
warnings.filterwarnings("ignore", category=DeprecationWarning)

np.random.seed(9)

def f(x):
    return np.sin(2 * np.pi * x)

# generate points used to plot
x_plot = np.linspace(0, 1, 100)

# generate points and keep a subset of them
n_samples = 100
X = np.random.uniform(0, 1, size=n_samples)[:, np.newaxis]
y = f(X) + np.random.normal(scale=0.3, size=n_samples)[:, np.newaxis]
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.8)

ax = plt.gca()
ax.plot(x_plot, f(x_plot), color='green')
ax.scatter(X_train, y_train, s=10)
ax.set_ylim((-2, 2))
ax.set_xlim((0, 1))
ax.set_ylabel('y')
ax.set_xlabel('x')
```

```
Populating the interactive namespace from numpy and matplotlib
use backports
```

Out[1]:

```
<matplotlib.text.Text at 0x5008e90>
```

Now let's see how different polynomials can approximate this curve.

In [2]:

```
def plot_approximation(est, ax, label=None):
    """Plot the approximation of ``est`` on axis ``ax``. """
    ax.plot(x_plot, f(x_plot), color='green')
    ax.scatter(X_train, y_train, s=10)
    ax.plot(x_plot, est.predict(x_plot[:, np.newaxis]), color='red', label=label)
    ax.set_ylim((-2, 2))
    ax.set_xlim((0, 1))
    ax.set_ylabel('y')
    ax.set_xlabel('x')
    ax.legend(loc='upper right')  #, fontsize='small')

fig, axes = plt.subplots(2, 2, figsize=(8, 5))
# fit different polynomials and plot approximations
for ax, degree in zip(axes.ravel(), [0, 1, 3, 9]):
    est = make_pipeline(PolynomialFeatures(degree), LinearRegression())
    est.fit(X_train, y_train)
    plot_approximation(est, ax, label='degree=%d' % degree)

plt.tight_layout()
```

In the plot above we see that the polynomial of degree zero is just a constant approximation, the polynomial of degree one fits a straight line, the polynomial of degree three nicely approximates the ground truth, and finally, the polynomial of degree nine has nearly zero training error but does a poor job approximating the ground truth because it already fits the variance induced by the random gaussian noise that we added to our data.

If we plot the training and testing error as a function of the degree of the polynomial we can see what's happening: the higher the degree of the polynomial (our proxy for model complexity), the lower the training error. The testing error decreases too, but it eventually reaches its minimum at a degree of three and then starts increasing at a degree of seven.

This phenomenon is called *overfitting*: the model is already so complex that it fits the idiosyncrasies of our training data, idiosyncrasies which limit the model's ability to generalize (as measured by the testing error).

In [3]:

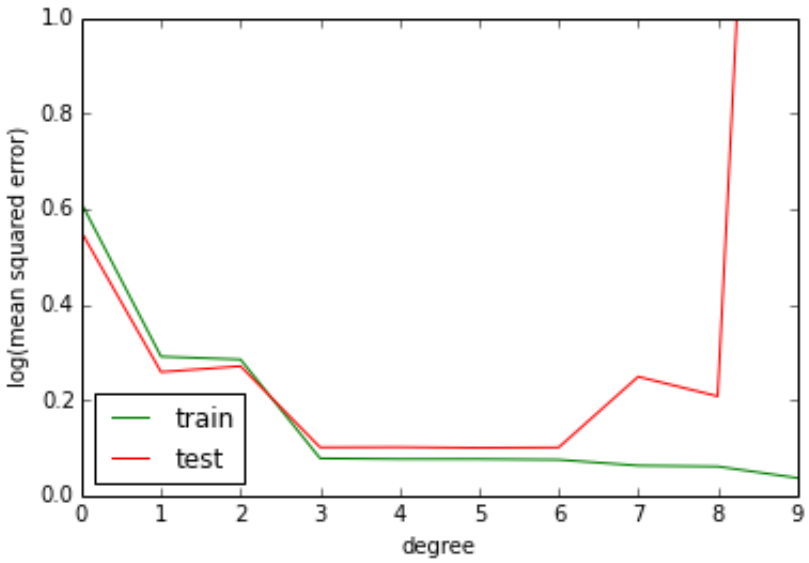
```
from sklearn.metrics import mean_squared_error

train_error = np.empty(10)
test_error = np.empty(10)
for degree in range(10):
    est = make_pipeline(PolynomialFeatures(degree), LinearRegression())
    est.fit(X_train, y_train)
    train_error[degree] = mean_squared_error(y_train, est.predict(X_train))
    test_error[degree] = mean_squared_error(y_test, est.predict(X_test))

plt.plot(np.arange(10), train_error, color='green', label='train')
plt.plot(np.arange(10), test_error, color='red', label='test')
plt.ylim((0.0, 1e0))
plt.ylabel('log(mean squared error)')
plt.xlabel('degree')
plt.legend(loc='lower left')
```

Out[3]:

```
<matplotlib.legend.Legend at 0x58d64d0>
```



(http://www.datarobot.com/wp-content/uploads/2014/03/reg-lin-reg-learn-curve.png)

In the above example, the optimal choice for the degree of the polynomial approximation would be between three and six. However, there is an alternative to manually selecting the degree of the polynomial: we can add a constraint to our linear regression model that constrains the magnitude of the coefficients in the regression model. This constraint is called the regularization term and the technique is often called shrinkage in the statistical community because it shrinks the coefficients towards zero. In the context of polynomial regression, constraining the magnitude of the regression coefficients effectively is a smoothness assumption: by constraining the L2 norm of the regression coefficients we express our preference for smooth functions rather than wiggly functions.

A popular regularized linear regression model is Ridge Regression. This adds the L2 norm of the coefficients to the ordinary least squares objective:

$$J(\boldsymbol{\beta}) = \frac{1}{n}\sum_{i=0}^{n}(y_i - \boldsymbol{\beta}^T\mathbf{x}_i')^2 + \alpha\|\boldsymbol{\beta}\|_2$$

where β is the vector of coefficients including the intercept term and $\mathbf{x}_i'$ is the vector of the predictors of the i-th data point including a constant predictor for the intercept. The L2 norm term is weighted by a regularization parameter `alpha`: if `alpha=0` then you recover the Ordinary Least Squares regression model. The larger the `alpha` the higher the smoothness constraint.

Below you can see the approximation of a `sklearn.linear_model.RidgeRegression` estimator fitting a polynomial of degree nine for various values of `alpha` (left) and the corresponding coefficient loadings (right). The smaller the value of `alpha` the higher the magnitude of the coefficients, so the functions we can model can be more and more wiggly.

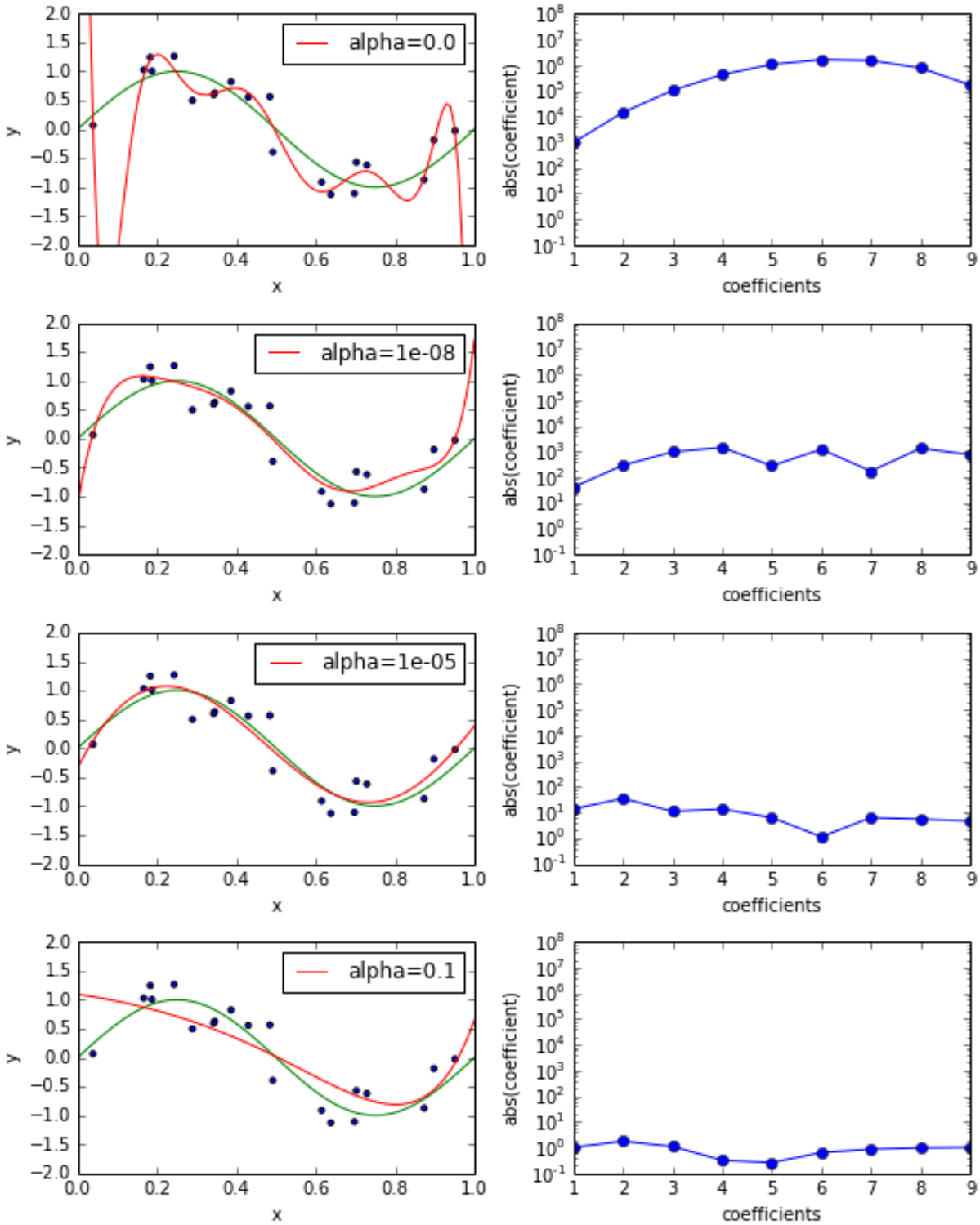
In [4]:

```
fig, ax_rows = plt.subplots(4, 2, figsize=(8, 10))

def plot_coefficients(est, ax, label=None, yscale='log'):
    coef = est.steps[-1][1].coef_.ravel()
    if yscale == 'log':
        ax.semilogy(np.abs(coef), marker='o', label=label)
        ax.set_ylim((1e-1, 1e8))
    else:
        ax.plot(np.abs(coef), marker='o', label=label)
    ax.set_ylabel('abs(coefficient)')
    ax.set_xlabel('coefficients')
    ax.set_xlim((1, 9))

degree = 9
alphas = [0.0, 1e-8, 1e-5, 1e-1]
for alpha, ax_row in zip(alphas, ax_rows):
    ax_left, ax_right = ax_row
    est = make_pipeline(PolynomialFeatures(degree), Ridge(alpha=alpha))
    est.fit(X_train, y_train)
    plot_approximation(est, ax_left, label='alpha=%r' % alpha)
    plot_coefficients(est, ax_right, label='Ridge(alpha=%r) coefficients' % alpha)

plt.tight_layout()
```



(http://www.datarobot.com/wp-content/uploads/2014/03/reg-lin-reg-reg.png)

Regularization techniques

In the above example we used Ridge Regression, a regularized linear regression technique that puts an L2 norm (http://mathworld.wolfram.com/L2-Norm.html) penalty on the regression coefficients. Another popular regularization technique is the LASSO, a technique which puts an L1 norm (http://mathworld.wolfram.com/L1-Norm.html) penalty instead. The difference between the two is that the LASSO leads to sparse solutions, driving most coefficients to zero, whereas Ridge Regression leads to dense solutions, in which most coefficients are non-zero. The intuition behind the sparseness property of the L1 norm penalty can be seen in the plot below. The plot

shows the value of the penalty in the coefficient space, here a space with two coefficients w_0 and w_1. The L2 penalty appears as a cone in this space whereas the L1 penalty is a diamond. The objective function of a regularized linear model is just the ordinary least squared solution plus the (weighted) penalty term (the point that minimizes the objective function is where those two error surfaces meet), so in the case of the L1 penalty this is usually at the spike of the diamond, a sparse solution because some coefficients are zero. For the L2 penalty, on the other hand, the optimal point generally has non-zero coefficients. Another popular regularization technique is the Elastic Net, the convex combination of the L2 norm and the L1 norm. It too leads to a sparse solution.

L2 and L1 regularization differ in how they cope with correlated predictors: L2 will divide the coefficient loading equally among them whereas L1 will place all the loading on one of them while shrinking the others towards zero. Elastic Net combines the advantages of both: it tends to either select a group of correlated predictors in which case it puts equal loading on all of them, or it completely shrinks the group.

Scikit-learn provides separate classes for LASSO and Elastic Net: `sklearn.linear_model.Lasso` and `sklearn.linear_model.ElasticNet`. In contrast to RidgeRegression, the solution for both LASSO and Elastic Net has to be computed numerically. The classes above use an optimization technique called coordinate descent (http://en.wikipedia.org/wiki/Coordinate_descent). Alterntively, you can also use the class `sklearn.linear_model.SGDRegressor` which uses stochastic gradient descent (http://en.wikipedia.org/wiki/Stochastic_gradient_descent) instead and often is more efficient for large-scale, high-dimensional and sparse data.

In [5]:

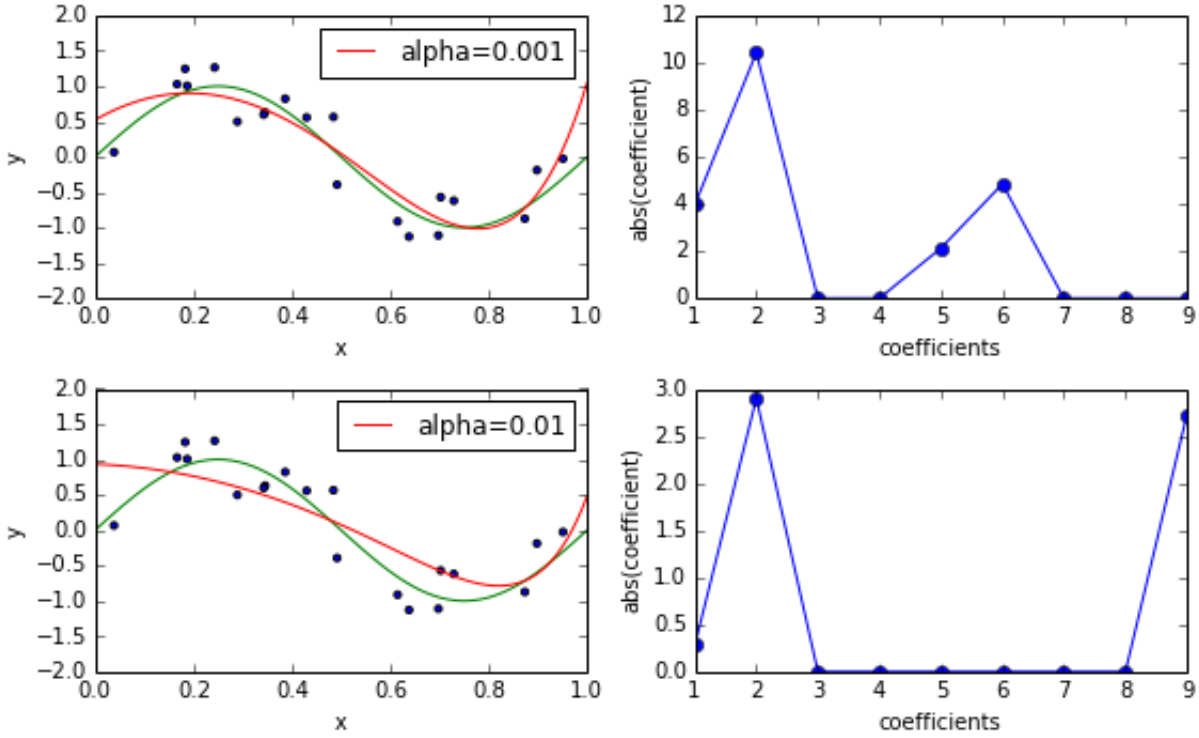
```
from sklearn.linear_model import Lasso

fig, ax_rows = plt.subplots(2, 2, figsize=(8, 5))

degree = 9
alphas = [1e-3, 1e-2]
for alpha, ax_row in zip(alphas, ax_rows):
    ax_left, ax_right = ax_row
    est = make_pipeline(PolynomialFeatures(degree), Lasso(alpha=alpha))
    est.fit(X_train, y_train)
    plot_approximation(est, ax_left, label='alpha=%r' % alpha)
    plot_coefficients(est, ax_right, label='Lasso(alpha=%r) coefficients' % alpha,
yscale=None)

plt.tight_layout()
```

```
/home/pprett/workspace/scikit-learn/sklearn/linear_model/coordinate_descent.py:48
1: UserWarning: Objective did not converge. You might want to increase the number
of iterations
  ' to increase the number of iterations')
```



(http://www.datarobot.com/wp-content/uploads/2014/03/reg-lin-reg-sparse-reg.png)

Regularization Path Plots

Another handy diagnostic tool for regularized linear regression is the use of so-called regularization path plots. These show the coefficient loading (y-axis) against the regularization parameter `alpha` (x-axis). Each (non-zero) coefficient is represented by a line in this space. The example (http://scikit-learn.org/dev/auto_examples/linear_model/plot_lasso_coordinate_descent_path.html) below is taken from the scikit-learn documentation. You can see that the smaller the `alpha` (i.e. the higher the `-log(alpha)`, the higher the magnitude of the coefficients and the more predictors selected). You can also see that the Elastic Net tends to select more predictors, distributing the loading evenly among them, whereas L1 tends to select fewer predictors.

Regularization path plots can be efficiently created using coordinate descent optimization methods but they are harder to create with (stochastic) gradient descent optimzation methods. Scikit-learn provides a number of convenience functions to create those plots for coordinate descent based regularized linear regression models: `sklearn.linear_model.lasso_path` and `sklearn.linear_model.enet_path`.

Download Notebook (https://s3.amazonaws.com/datarobotblog/notebooks/regularized-linear-regression.ipynb)
View on NBViewer (http://nbviewer.ipython.org/urls/s3.amazonaws.com/datarobotblog/notebooks/regularized-linear-regression.ipynb)

This post was written by Peter Prettenhofer and Mark Steadman. Please post any feedback, comments, or questions below or send us an email at <firstname>@datarobot.com.

6 Responses to “Regularized Linear Regression with scikit-learn”

Aneesh

Great post. Really helpful for someone coming from Matlab who is transitioning to scikit-learn! Would love to read about more scikit-learn use cases!

Reply (http://www.datarobot.com/blog/regularized-linear-regression-with-scikit-learn/?replytocom=1665#respond)

Ashwath

It is mentioned to use use backports for sklearn 1.4 but sklearn is at version 0.14 now.

Also, 'PolynomialFeatures' are not available in the current stable version. How do I get the sklearn-backports? It doesn't look like a PyPI package?

Thanks.

Reply (http://www.datarobot.com/blog/regularized-linear-regression-with-scikit-learn/?replytocom=4947#respond)

Peter Prettenhofer

Thanks for pointing this out Ashwath.

I've updated the code snippet; the backport of the polynomial module is available here: https://s3.amazonaws.com/datarobotblog/notebooks/sklearn_backports.py (https://s3.amazonaws.com/datarobotblog/notebooks/sklearn_backports.py)

I was expecting that sklearn 0.15 will be released shortly after writing the blog post — I was wrong.

Reply (http://www.datarobot.com/blog/regularized-linear-regression-with-scikit-learn/?replytocom=4949#respond)

Xan

Very helpful. For the ridge regression, do you know if there is a way to keep the intercept term from being regularized? I usually do not want the intercept coefficient to be diluted. It would be great if I could specify different alphas for each coefficient separately.

Reply (http://www.datarobot.com/blog/regularized-linear-regression-with-scikit-learn/?replytocom=17006#respond)

Moustafa Alzantot

Reply (http://www.datarobot.com/blog/regularized-linear-regression-with-scikit-learn/?replytocom=73648#respond)

very nice tutorial ! thanks for posting this !

Ted Kwartler (http://www.datarobot.com)

Reply (http://www.datarobot.com/blog/regularized-linear-regression-with-scikit-learn/?replytocom=73792#respond)

Moustafa- thanks for the feedback!

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