gbm_solution

July 15, 2019

0.1 Gradient Boosting

In this notebook, you will use scikit-learn's regression trees and implement the gradient boosting algorithm for least squares regression. In particular, you will:

1. Implement gradient boosting with shrinkage and evaluate its performance on the boston housing data set.
2. Investigate the effect of number of iterations and tree depth.
3. Plot the additive structure of gradient boosting.

The exercise is mostly based on the lecture and the following book:
T. Hastie, R. Tibshirani, and J. Friedman: *The Elements for Statistical Learning*, 2001
As usual, some setup first:

```
In [1]: import sklearn.cross_validation
        import sklearn.datasets
        import sklearn.dummy
        import sklearn.tree
        import sklearn.base
        import sklearn.metrics
        import sklearn.ensemble

        import numpy as np

        import matplotlib.pyplot as plt
```

```
/home/eggenspk/anaconda3/envs/general_36/lib/python3.6/site-packages/sklearn/cross_validation.
  "This module will be removed in 0.20.", DeprecationWarning)
/home/eggenspk/anaconda3/envs/general_36/lib/python3.6/site-packages/sklearn/ensemble/weight_b
  from numpy.core.umath_tests import inner1d
```

```
In [2]: # Load the boston housing dataset
        def create_dataset():

            boston = sklearn.datasets.load_boston()
            X = boston.data
            y = boston.target
            X_train, X_test, y_train, y_test = \
                sklearn.cross_validation.train_test_split(X, y, random_state=1)
            return X_train, y_train, X_test, y_test
```

```
In [3]: class GradientBoosting(object):

            def __init__(self, iterations, learning_rate=1.0):
                # Some global variables
                self.iterations = iterations
                self.classifiers = list()
                self.weak_learner = sklearn.tree.\
                    DecisionTreeRegressor(max_depth=1)
                self.learning_rate = learning_rate

            # derivative of L2 loss
            def _delta_l(self, y_true, f_of_x):
                return y_true - f_of_x

            def fit(self, X, y):
                # 1. Initialize f_0
                # hint: Scikit-learn offers dummy predictors
                # (e.g. DummyRegressor), which return constant
                # predictions according to a simple, user-defined rule
                f_0 = sklearn.dummy.DummyRegressor(strategy='mean')
                f_0.fit(X, y)
                self.classifiers.append(f_0)

                f_of_x = f_0.predict(X)

                # 2. For m = 1 to m
                for iteration in range(self.iterations):

                    # 2.a) compute pseudo residuals
                    generalized_residuals = self._delta_l(y, f_of_x)

                    # 2.b) fit regression tree to the residuals
                    # 2.c) update terminal region: not necessary for
                    #       squared loss
                    f_m = sklearn.base.clone(self.weak_learner)
                    f_m.fit(X, generalized_residuals)

                    # 2.d) update f_of_x
                    f_of_x += self.learning_rate*f_m.predict(X)
                    self.classifiers.append(f_m)

                return self

            def predict(self, X):
```

```
        predictions = self.classifiers[0].predict(X)
        for classifier in self.classifiers[1:]:
            predictions += self.learning_rate*classifier.predict(X)

        return predictions

    def staged_predict(self, X):
        # returns predictions for X for all iterations
        # this is for convenience to simplify computing
        # train/test error for all models

        staged_predictions = []
        pred = self.classifiers[0].predict(X)
        staged_predictions.append(pred.copy())
        for classifier in self.classifiers[1:]:
            pred += self.learning_rate*classifier.predict(X)
            staged_prediction = pred.copy()
            staged_predictions.append(staged_prediction)

        return staged_predictions
```

Note: As you use *squared loss* there is no need to update the terminal regions in each leaf as the values in the leaves of decision trees already are optimal constant to minimize squared loss. With other loss functions you would need to update the leaf-values, such as done in sklearn:

https://github.com/scikit-learn/scikit-learn/blob/51a765a/sklearn/ensemble/gradient_boosting.py#L792

such as minimizing the least absolute error here:

https://github.com/scikit-learn/scikit-learn/blob/51a765a/sklearn/ensemble/gradient_boosting.py#L321

0.1.1 Test your implementation

Now, you have a working implementation of the gradient boosting algorithm.

To test your algorithm for correctness you can compare to sklearn's gradient boosting implementation which should yield the same output as your implementation:

```
In [4]: # Use this cell to test whether your implementation is correct

        gbm = GradientBoosting(iterations=400, learning_rate=1.0)
        sk_gbm = sklearn.ensemble.GradientBoostingRegressor(
            n_estimators=400, learning_rate=1.0, max_depth=1)

        # Get data
        X_train, y_train, X_test, y_test = create_dataset()

        # Fit model
        gbm.fit(X_train, y_train)
        sk_gbm.fit(X_train, y_train)

        # Predict
        pred = gbm.predict(X_test)
        pred_sk = sk_gbm.predict(X_test)

        print("Difference: %d" % np.sum([pred - pred_sk]))
```

```
Difference: 0
```

0.1.2 Add shrinkage

The scikit-learn implementation offers a parameter 'learning_rate' which implements skrinkage, such that the contribution of each model is shrinked. This means the adaption to the target function is slowed down and thus prevents gradient boosting from overfitting. Changing line (d) in the Pseudocode (see Algorithm 10.3 *Gradient Tree Boosting Algorithm*) from
$f_m(x) = f_{m-1}(x) + \sum_{j=1}^{J_m} \gamma_{jm} \mathbf{I}(x \in R_{jm})$
to
$f_m(x) = f_{m-1}(x) + \nu \sum_{j=1}^{J_m} \gamma_{jm} \mathbf{I}(x \in R_{jm})$
will do this. Add a learning rate to your implementation of Gradient Boosting.

0.1.3 Playground

Next, you can now play around with AdaBoost's hyperparameters. Here are some suggestions to try:

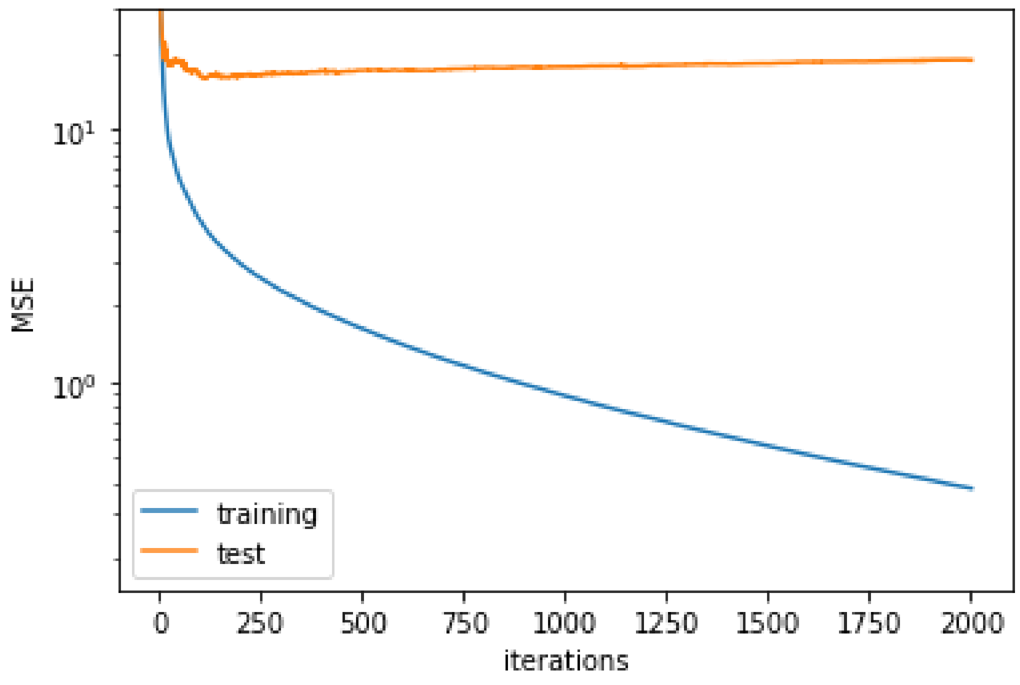
- Investigate the number of iterations that are needed to start overfitting.
- Add some noise on the targets and try again
- Investigate the effect of the tree depth
- Investigate effect of shrinkage

But first you should implement a plotting function to show train/test error over time:

```
In [10]: def plot_train_test_error(model, X_train, y_train, X_test, y_test):
             ''' Shows a plot with train/test error over iterations

             model (GBM): trained GBM algorithm
             X_train (array): [#samples, #features]
             y_train (array): [#samples, ]
             X_test (array): [#samples, #features]
             y_test (array): [#samples, ]
             '''
             # YOUR TURN

             # Loop over all predictions and compute the mean squared error

             y_pred_train = model.staged_predict(X_train)
             training_errors = [sklearn.metrics.mean_squared_error(y_train, y_pred)
                                for y_pred in y_pred_train]

             y_pred_test = model.staged_predict(X_test)
```

```
    test_errors = [sklearn.metrics.mean_squared_error(y_test, y_pred)
                   for y_pred in y_pred_test]

    # Plot results
    x_values = np.arange(1, len(training_errors) + 1)

    plt.plot(x_values, training_errors, label="training")
    plt.plot(x_values, test_errors, label="test")
    plt.xlabel("iterations")
    plt.ylabel("MSE")
    plt.legend(loc="best")

    #plt.show()
```

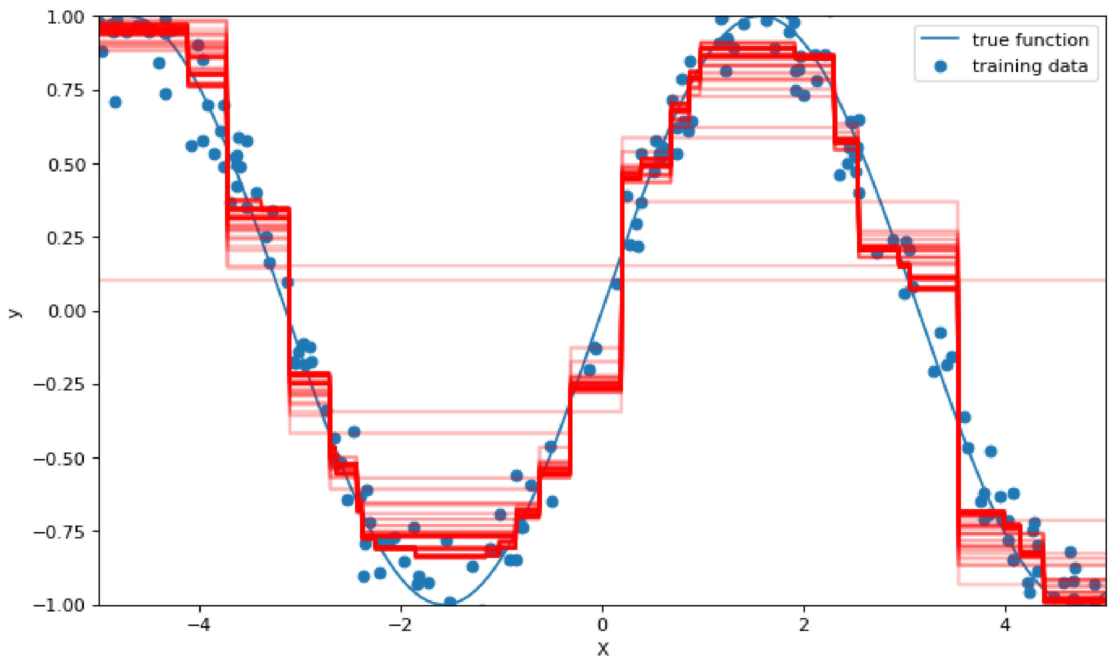
```
In [14]: # The train and test error diverge after roughly ~15 iterations.
         # While the training error constantly decreases, test error raises
         # after ~200 iterations. With deeper trees, the test error can be
         # decreased to zero for the price of earlier overfitting on the test set.
         # Adding noise with std=1 does harm the performance only slightly
         # Adding noise with std=2 harms the performance quite a lot
         # Adding more noise results also in increased overfitting
         # A lower learning rate prevents overfitting and training error does
         # not decrease to 0

         # YOUR TURN

         # Get data
         X_train, y_train, X_test, y_test = create_dataset()

         # Instantiate model
         gbm = GradientBoosting(iterations=2000, learning_rate=1)

         # Fit model
         gbm.fit(X_train, y_train)
         pred = gbm.predict(X_test)

         # Evaluate model
         plot_train_test_error(gbm, X_train, y_train, X_test, y_test)
         plt.ylim([0.15, 30])
         plt.yscale('log')
```



0.1.4 Plot individual models

Finally, it's time to investigate the additive nature of gradient boosting. For this, we plot the prediction of the gradient boosting model for a sine curve after different amounts of iterations

```
In [27]: # Here's some training data:
         np.random.seed(1)
         num_data_points = 200
         lower_bound = -5
         upper_bound = 5
         X = np.random.uniform(lower_bound, upper_bound, num_data_points)
         X = X.reshape((-1, 1))
         y = (np.sin(X) + np.random.randn(num_data_points).reshape((-1, 1)) * 0.1)
         y = y.ravel()

         true_function_X = np.arange(lower_bound, upper_bound, 0.01)
         true_function_X = true_function_X.reshape((-1, 1))

         plt.figure(num=None, figsize=(10, 6), dpi=80, facecolor='w',
                    edgecolor='k')
         plt.scatter(X.ravel(), y, label="training data")
         plt.plot(true_function_X, np.sin(true_function_X),
                  label='true function')
         plt.xlabel("X")
         plt.ylabel("y")
         plt.legend(loc="best")
         plt.ylim([-1, 1])
         plt.xlim([lower_bound, upper_bound])

         # YOUR TURN
         # Plot a line for each model
         iterations = 50
         num_curves = 25

         gbm = GradientBoosting(iterations=iterations,)
         gbm.fit(X, y)
         staged_predictions = gbm.staged_predict(true_function_X)

         for i, prediction in enumerate(staged_predictions):
             if int(iterations / num_curves) != 0 and \
                  i % int(iterations / num_curves) != 0:
                 continue

             alpha = 0.2 + (i / len(staged_predictions) / 1.8)
             plt.plot(true_function_X, prediction, color='red',
                      linewidth=2, alpha=alpha)

         plt.show()
```


y
X
true function
training data