lof

April 23, 2014

1 Improving performance of Local outlier factor with KD-Trees

Local outlier factor (LOF) is an outlier detection algorithm, that detects outliers based on comparing local density of data instance with its neighbors. It does so to decide if data instance belongs to region of similar density. It can detect an outlier in a dataset, for which number of clusters is unknown, and clusters are of different density and size. It's inspired from KNN (K-Nearest Neighbors) algorithm, and is widely used. There is a R implemantation available.

The naive approach to do this is to form all pair euclidan distance matrix, and then run knn query to proceed further. But this approach just sucks, as it is $\Theta(n^2)$ in terms of both space and time complexity. But, this can be improvd with KDTrees., and already its implementation exists in python, thanks to scipy, so lets use this to find outliers.

Synthetic dataset

```
In [229]: %pylab inline
          import numpy as np
          np.random.seed(2) # to reproduce the result
```

```
Populating the interactive namespace from numpy and matplotlib

WARNING: pylab import has clobbered these variables: ['dist']
`%pylab --no-import-all` prevents importing * from pylab and numpy
```

```
In [230]: dim = 2 # number of dimensions of dataset = 2
          # cluster of normal random variable moderately dense
          data1 = np.random.np.random.multivariate_normal([0, 1500], [[100000, 0], [0, 100000]], 2000)

          # very dense
          data2 = np.random.np.random.multivariate_normal([2000, 0], [[10000, 0], [0, 10000]], 2500)

          # sparse
          data3 = np.random.np.random.multivariate_normal([2500, 2500], [[100000, 0], [0, 100000]], 500

          # mix the three dataset and shuffle
          data = np.vstack((np.vstack((data1, data2)), data3))
          np.random.shuffle(data)

          # add some noise : zipf is skewed distribution and can have extreme values(outliers)
          zipf_alpha = 2.25
          noise = np.random.zipf(zipf_alpha, (5000,dim)) * np.sign((np.random.randint(2, size = (5000, d
          data += noise
```

Naive approach to LOF Pairwise Euclidean distance calculation with DistanceMetric implementation in scikit-learn. In this, we just compute all-pair euclidean distance, i.e. $d(i,j) = \|x(i) - x(j)\|_2$.

In [231]:
```
from sklearn.neighbors import DistanceMetric
 # distance between points
import time
tic = time.time()
dist = DistanceMetric.get_metric('euclidean').pairwise(data)
print '++ took %g msecs for Distance computation' %  ((time.time() - tic)* 1000)
```

```
++ took 740 msecs for Distance computation
```

Performing KNN query.In this step, the nearest k neighbors are identified $N_k(i)$, and radius is the distance of k-th rearest neighbor of a datapoint.

$$r(i) = \max_{k \in N_k(i)} d(i,k)$$

In [232]:
```
tic = time.time()
k = 17 # number of neighbors to consider
# get the radius for each point in dataset (distance to kth nearest neighbor)
# radius is the distance of kth nearest point for each point in dataset
idx_knn = np.argsort(dist, axis=1)[:,1 : k + 1] # by row' get k nearest neighbour
radius = np.linalg.norm(data - data[idx_knn[:, -1]], axis = 1) # radius
print '+++ took %g msecs for KNN Querying' %  ((time.time() - tic)* 1000)
```

```
+++ took 4800 msecs for KNN Querying
```

Then LRD(Local Reachability distance) is calculated. For this, first reach distance $rd(i,j)$ is computed between point concern $x(i)$ and its neighbors \$ j:j∈ $N\_k(i)$, which is the maximum of euclidean distance or radius $r(i)\$ of point concerned. Then, LRD is the inverse of mean of reach distance of all k - neighbors of each point. rd(i,j) = \max\{d(i,j), r(i)\} for\ j \in N_k(i)$

$$LRD(i) = \frac{|N_k(i)|}{\sum_{j \in N_k(i)} rd(i,j)}$$

In [233]:
```
# calculate the local reachability density
tic = time.time()
LRD = []
for i in range(idx_knn.shape[0]):
    LRD.append(np.mean(np.maximum(dist[i, idx_knn[i]], radius[idx_knn[i]])))
print '++++ took %g msecs for LRD computation' %  ((time.time() - tic)* 1000)
```

```
++++ took 429 msecs for LRD computation
```

finally, the outlier score LOF is calsulated.

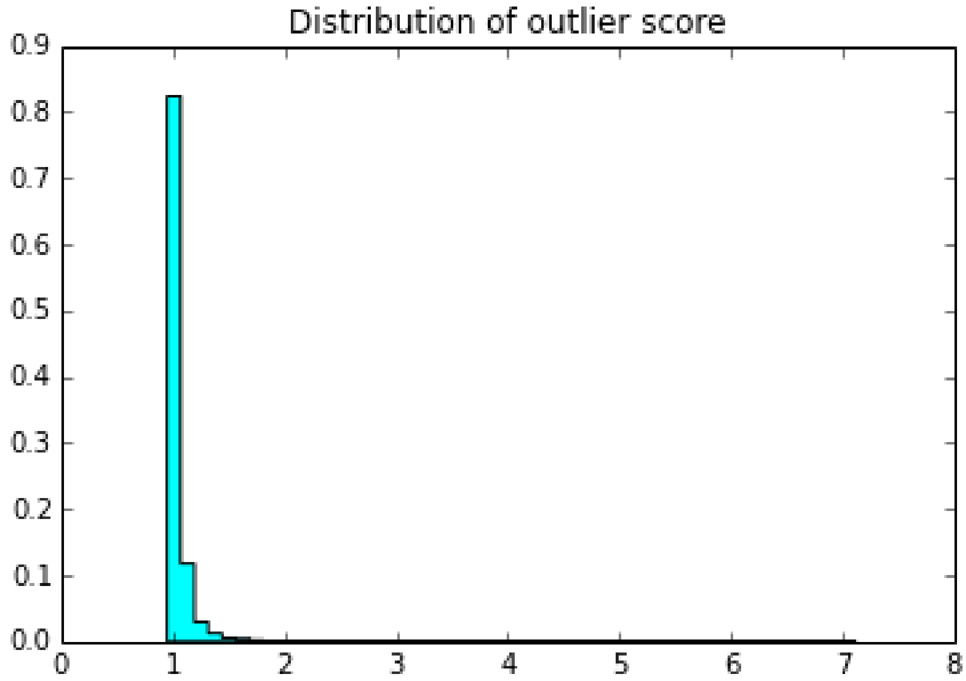
$$LOF(i) = \frac{\sum_{j \in N_k(i)} \frac{LRD(j)}{LRD(i)}}{|N_k(i)|}$$

In [234]:
```
# calculating the outlier score
tic = time.time()
rho = 1. / np.array(LRD) # inverse of density
outlier_score = np.sum(rho[idx_knn], axis = 1)/ np.array(rho, dtype = np.float16)
outlier_score *= 1./k
print '+++++ took %g msecs for Outlier scoring' %  ((time.time() - tic)* 1000)
```

```
+++++ took 9.99999 msecs for Outlier scoring
```

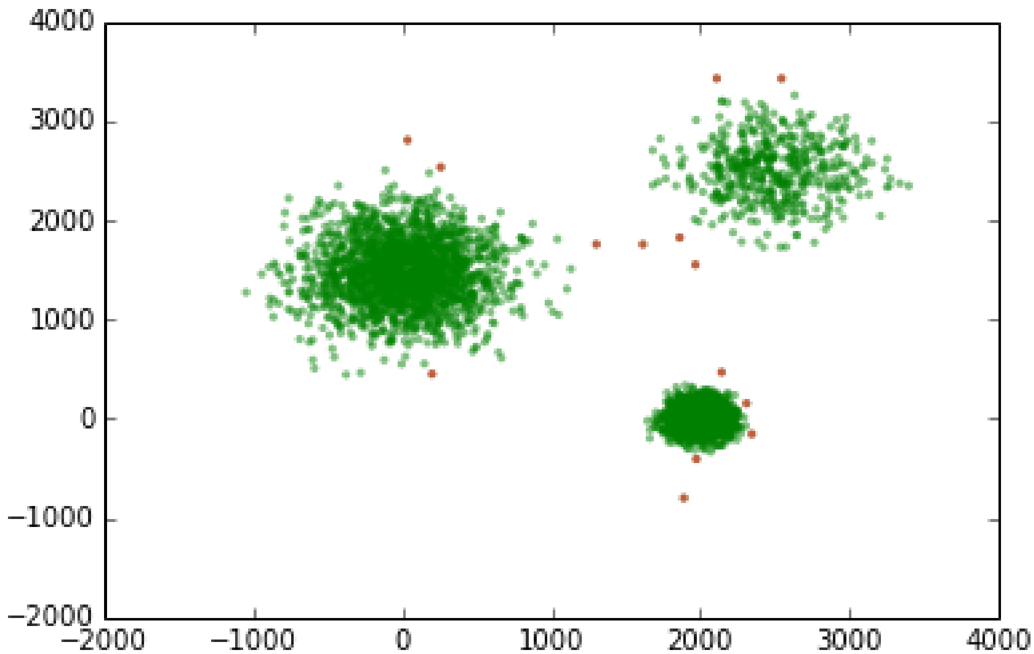
Now lets se the histogram of Outlier score, to choose the optimal threshold to decid weather a data-point is outlier is not.

```
In [235]: weights = np.ones_like(outlier_score)/outlier_score.shape[0] # to normalize the histogram to p
          hist(outlier_score, bins = 50, weights = weights, histtype = 'stepfilled', color = 'cyan')
          title('Distribution of outlier score')

Out[235]: <matplotlib.text.Text at 0x36030588>
```



It can be observd that, the optimal outlier score threshold to decide weather a data-point is outlier is outlier or not is around 2 for most of the cases, so lets use it to see our sesults.

```
In [236]: threshold = 2.
          # plot non outliers as green
          scatter(data[:, 0], data[:, 1], c = 'green', s = 10, edgecolors='None', alpha=0.5)
          # find the outliers and plot te outliers
          idx = np.where(outlier_score > threshold)
          scatter(data[idx, 0], data[idx, 1], c = 'red', s = 10, edgecolors='None', alpha=0.5)

Out[236]: <matplotlib.collections.PathCollection at 0x3640e6a0>
```



We have seen the results of LOF with naive approachfor KNN queries. Now lets see optimisations with KD-Trees.

Using KD Trees KD-Trees insertion and KNN query.

```
In [239]: from sklearn.neighbors import KDTree as Tree
          tic = time.time()
          BT = Tree(data, leaf_size=5, p=2)
          # Query for k nearest, k + 1 because one of the returnee is self
          dx, idx_knn = BT.query(data[:, :], k = k + 1)

          print '++ took %g msecs for Tree KNN Querying' %  ((time.time() - tic)* 1000)
```

```
++ took 122 msecs for Tree KNN Querying
```

LRD computation.

```
In [240]: tic = time.time()
          dx, idx_knn = dx[:, 1:], idx_knn[:, 1:]
          # get the radius for each point in dataset
          # radius is the distance of kth nearest point for each point in dataset
          radius = dx[:, -1]
          # calculate the local reachability density
          LRD = np.mean(np.maximum(dx, radius[idx_knn]), axis = 1)

          print '++ took %g msecs for LRD computation' %  ((time.time() - tic)* 1000)
```

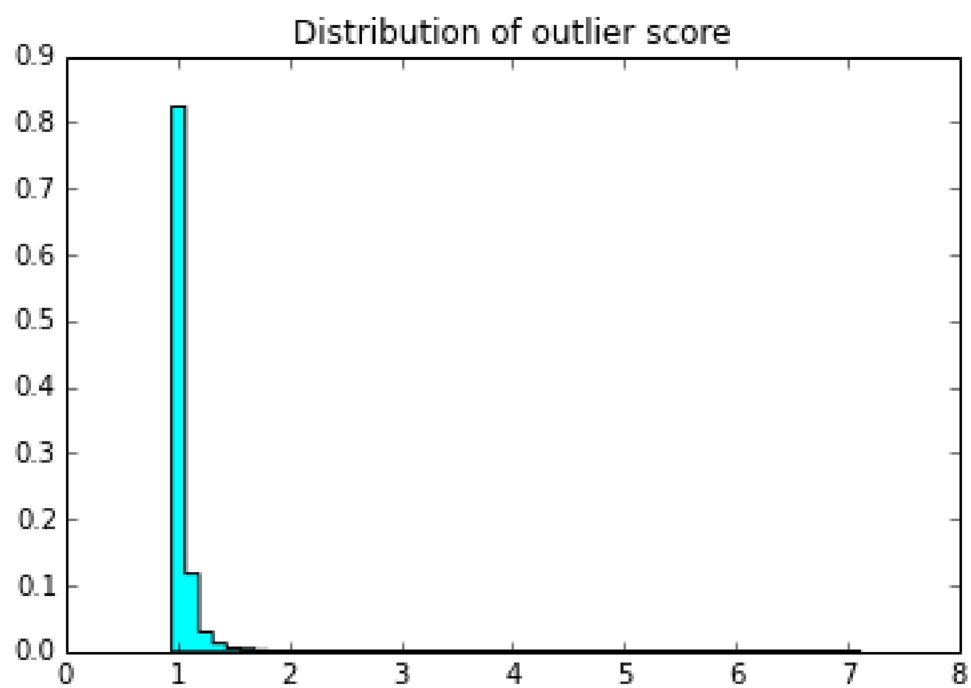
```
++ took 8.99982 msecs for LRD computation
```

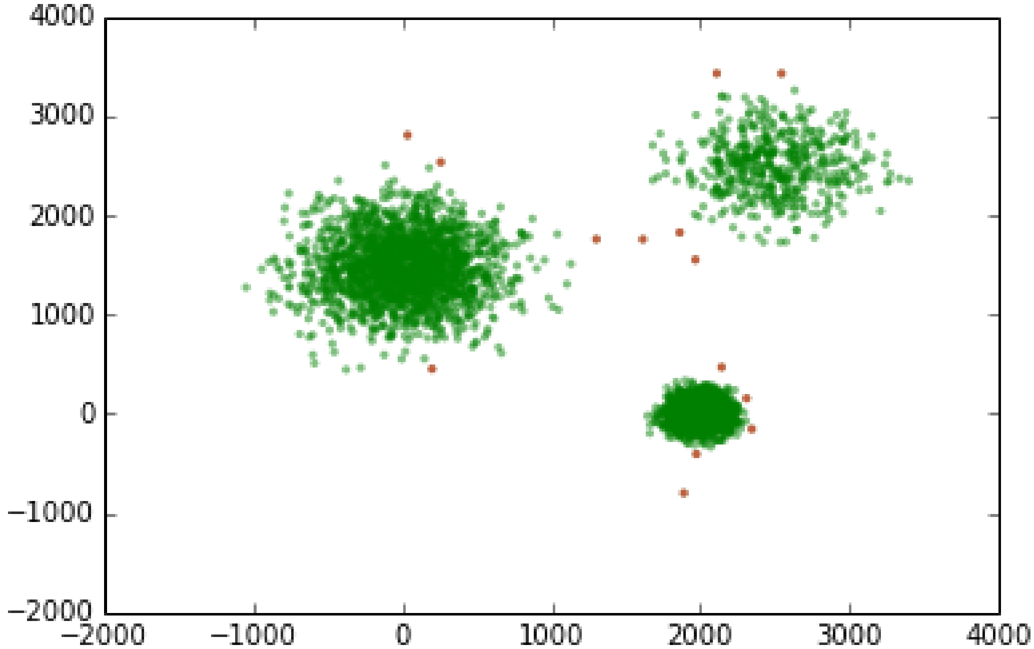
Now, rest is same, so, i'm just replicating the rsult for completion.

In [241]:
```python
# calculating the outlier score
tic = time.time()
rho = 1. / np.array(LRD) # inverse of density
outlier_score = np.sum(rho[idx_knn], axis = 1)/ np.array(rho, dtype = np.float16)
outlier_score *= 1./k
print '+++++ took %g msecs for Outlier scoring' %  ((time.time() - tic)* 1000)

# ploting the histogram of outlier score
weights = np.ones_like(outlier_score)/outlier_score.shape[0] # to normalize the histogram to
hist(outlier_score, bins = 50, weights = weights, histtype = 'stepfilled', color = 'cyan')
title('Distribution of outlier score')

#plotting the result
threshold = 2.
# plot non outliers as green
figure()
scatter(data[:, 0], data[:, 1], c = 'green', s = 10, edgecolors='None', alpha=0.5)
# find the outliers and plot te outliers
idx = np.where(outlier_score > threshold)
scatter(data[idx, 0], data[idx, 1], c = 'red', s = 10, edgecolors='None', alpha=0.5)
```

```
+++++ took 4.00019 msecs for Outlier scoring
```

Out[241]:
```
<matplotlib.collections.PathCollection at 0x36ad0b38>
```





The results are same, and should be.

Putting everything together Lets create a class, to combine evrything together. It will be important in evaluating performance. From above results, we note that the most time is spent for KNN querying.

```
In [225]: import numpy as np
          import matplotlib.pyplot as plt
          import sys
          from sklearn.neighbors import DistanceMetric
          from sklearn.datasets import make_blobs
          from sklearn.neighbors import KDTree as Tree

          def exit():
              sys.exit()

          class LOF:
              def __init__(self, k = 3):
                  self.k = k

              # a function to create synthetic test data
              def generate_data(self, n = 500, dim = 3):

                  n1, n2 = n / 3, n / 5
                  n3 = n - n1 - n2

                  # cluster of gaussian random data
                  data1, _ = make_blobs(n1, dim, centers= 3)

                  # cluster of uniform random variable
                  data2 = np.random.uniform(0, 25, size = (n2, dim))
```

```
        # cluster of dense uniform random variable
        data3 = np.random.uniform(100, 200, size = (n3, dim))

        # mix the three dataset
        self.data = np.vstack((np.vstack((data1, data2)), data3))
        np.random.shuffle(self.data)

        # add some noise : zipf is skewed distribution
        zipf_alpha = 2.5
        noise = np.random.zipf(zipf_alpha, (n,dim)) * \
                    np.sign((np.random.randint(2, size = (n, dim)) - 0.5))
        self.data += noise

    # KNN querying with naive approach
    def _knn_naive(self):

        # distance between points
        # import time
        tic = time.time()
        dist = DistanceMetric.get_metric('euclidean').pairwise(self.data)
        # print '++ took %g msecs for Distance computation' %  ((time.time() - tic)* 1000)
        tic = time.time()
        # get the radius for each point in dataset (distance to kth nearest neighbor)
        # radius is the distance of kth nearest point for each point in dataset
        self.idx_knn = np.argsort(dist, axis=1)[:,1 : self.k + 1] # by row' get k nearest nei
        radius = np.linalg.norm(self.data - self.data[self.idx_knn[:, -1]], axis = 1) # radiu
        # print '+++ took %g msecs for KNN Querying' %  ((time.time() - tic)* 1000)
        # calculate the local reachability density
        LRD = []
        for i in range(self.idx_knn.shape[0]):
            LRD.append(np.mean(np.maximum(dist[i, self.idx_knn[i]], radius[self.idx_knn[i]])))
        return np.array(LRD)

    # knn querying with KDTrees
    def _knn_tree(self):

        #import time
        # tic = time.time()
        BT = Tree(self.data, leaf_size=5, p=2)

        # Query for k nearest, k + 1 because one of the returnee is self
        dx, self.idx_knn = BT.query(self.data[:, :], k = self.k + 1)

        # print '++ took %g msecs for Tree KNN Querying' %  ((time.time() - tic)* 1000)

        dx, self.idx_knn = dx[:, 1:], self.idx_knn[:, 1:]
        # get the radius for each point in dataset
        # radius is the distance of kth nearest point for each point in dataset
        radius = dx[:, -1]
        # calculate the local reachability density
        LRD = np.mean(np.maximum(dx, radius[self.idx_knn]), axis = 1)
        return LRD
```

```
def train(self, data = None, method = 'Naive') :

    # check if dataset is provided for training
    try:
        assert data != None and data.shape[0]
        self.data = data
        n = self.data.shape[0] # number of data points

    except AssertionError:
        try:
            n = self.data.shape[0] # number of data points
        except AttributeError:
            print 'No data to fit the model, please provide data or call generate_data me
            exit()
    try:
        assert method.lower() in ['naive', 'n', 'tree', 't']
    except AssertionError:
        print 'Method must be Naive|n or tree|t'
        exit()

    # find the rho, which is inverse of  LRD
    if method.lower() in ['naive', 'n']:
        rho = 1./ self._knn_naive()

    elif method.lower() in ['tree', 't']:
        rho = 1./ self._knn_tree()

    self.score = np.sum(rho[self.idx_knn], axis = 1)/ np.array(rho, dtype = np.float16)
    self.score *= 1./self.k

def plot(self, threshold = None):

    # set the threshold
    if not threshold:
        from scipy.stats.mstats import mquantiles
        threshold = max(mquantiles(self.score, prob = 0.95), 2.)
    self.threshold = threshold
    # reduce data to 2D if required
    if self.data.shape[1] > 2:
        from sklearn.decomposition import PCA
        pca = PCA(n_components = 2)
        self.data = pca.fit_transform(self.data)

    # plot non outliers as green
    plt.figure()
    plt.scatter(self.data[:, 0], self.data[:, 1], c = 'green', s = 10, edgecolors='None',

    # find the outliers and plot te outliers
    idx = np.where(self.score > self.threshold)
    plt.scatter(self.data[idx, 0], self.data[idx, 1], c = 'red', s = 10, edgecolors='None
    plt.legend(['Normal', 'Outliers'])

    # plot the distribution of outlier score
    plt.figure()
```

```
            weights = np.ones_like(self.score)/self.score.shape[0]
            plt.hist(self.score, bins = 25, weights = weights, histtype = 'stepfilled', color = '
            plt.title('Distribution of outlier score')
```

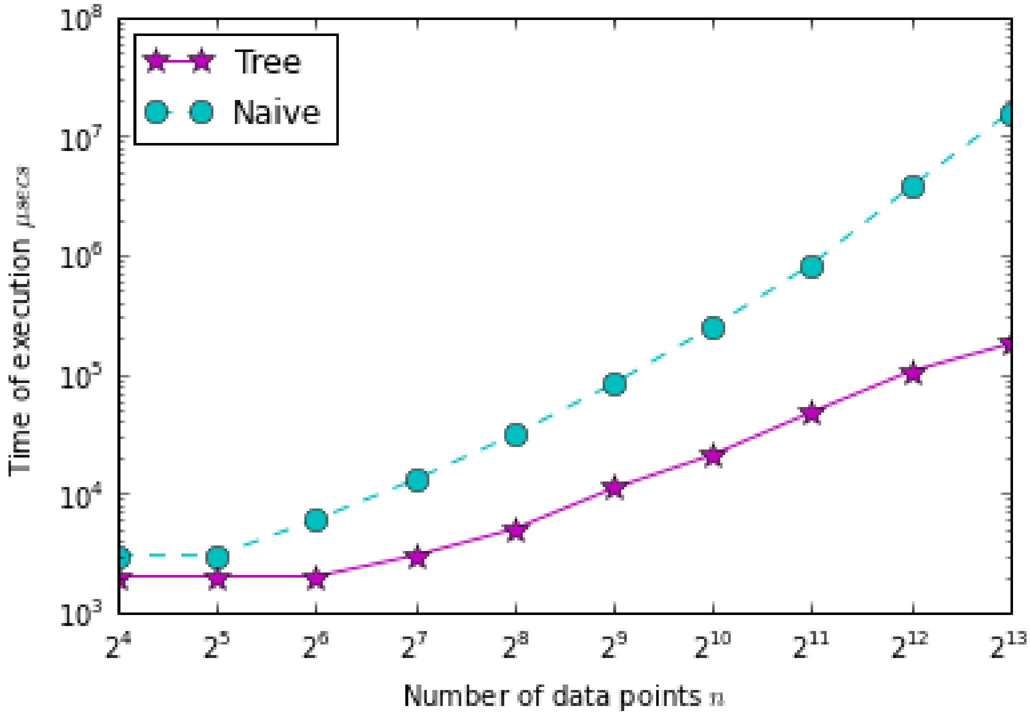
Performance Evaluation Lets create a function to evaluate te performance.

```
In [226]: def perf_test(n_list = None, methods = ['Tree', 'Naive'], plot = False):

              import time
              if not n_list: n_list = [2 ** i for i in range(7, 14)]
              result = []
              result.append(n_list)
              for m in methods:
                  temp = []
                  for n in n_list:
                      tic = time.time()
                      lof = LOF(k = 5)
                      lof.generate_data(n = n, dim = 2)
                      lof.train(method = m)
                      temp.append(1000000 * (time.time()-tic))
                      print 'Took %g msecs with %s method for %d datapoints' % \
                          ((time.time() - tic) * 1000, m, n)
                  result.append(temp)
              if plot:
                  fig, ax = plt.subplots()
                  ax.set_xscale('log', basex=2)
                  ax.set_yscale('log', basey=10)

                  plt.plot(result[0], result[1], 'm*-', ms = 10, mec = None)
                  try :
                      plt.plot(result[0], result[2], 'co--', ms = 8, mec = None)
                  except IndexError:
                      pass
                  plt.xlabel('Number of data points $n$')
                  plt.ylabel('Time of execution $\mu secs$')
                  plt.legend(methods, 'upper left')
                  plt.show()
```

Now, lets compare the performace of 2 methods- Naive and KDTree implementations.

```
In [243]: perf_test(methods = ['Tree', 'Naive'], n_list = [2 ** i for i in range(4, 14)], plot = True)

Took 2.00009 msecs with Tree method for 16 datapoints
Took 1.99986 msecs with Tree method for 32 datapoints
Took 2.00009 msecs with Tree method for 64 datapoints
Took 3.00002 msecs with Tree method for 128 datapoints
Took 4.99988 msecs with Tree method for 256 datapoints
Took 11.0002 msecs with Tree method for 512 datapoints
Took 20.9999 msecs with Tree method for 1024 datapoints
Took 48.0001 msecs with Tree method for 2048 datapoints
Took 106 msecs with Tree method for 4096 datapoints
Took 179 msecs with Tree method for 8192 datapoints
Took 3.00002 msecs with Naive method for 16 datapoints
Took 3.00002 msecs with Naive method for 32 datapoints
Took 6.00004 msecs with Naive method for 64 datapoints
```

```
Took 13 msecs with Naive method for 128 datapoints
Took 30.9999 msecs with Naive method for 256 datapoints
Took 82.9999 msecs with Naive method for 512 datapoints
Took 249 msecs with Naive method for 1024 datapoints
Took 834 msecs with Naive method for 2048 datapoints
Took 3734 msecs with Naive method for 4096 datapoints
Took 15796 msecs with Naive method for 8192 datapoints
```

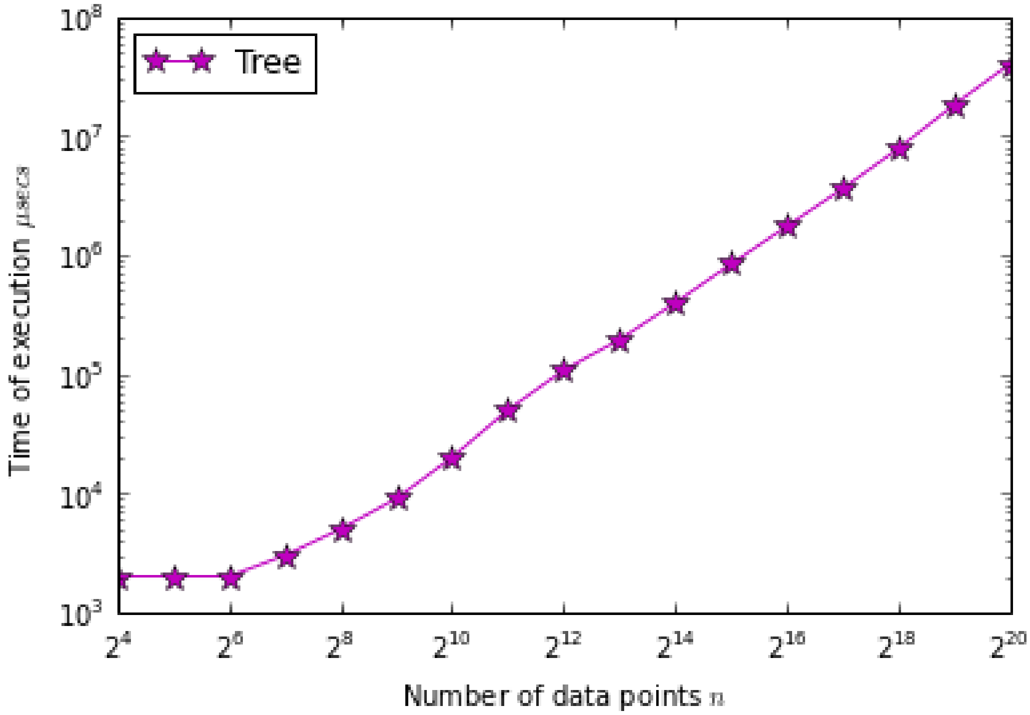


We see that KDTree outperforms Naive method for narge n, but it may not do well for small number of datasets. In my PC, i cannot run Naive method beyond 2^{13} datapoints, or else i receie MemoryError. So, lets evauate te performance of KDTrees upto 1Million datapoints.

```
In [244]: perf_test(methods = ['Tree'], n_list = [2 ** i for i in range(4, 21)], plot = True)
```

```
Took 2.00009 msecs with Tree method for 16 datapoints
Took 2.00009 msecs with Tree method for 32 datapoints
Took 1.99986 msecs with Tree method for 64 datapoints
Took 3.00002 msecs with Tree method for 128 datapoints
Took 6.00004 msecs with Tree method for 256 datapoints
Took 9.00006 msecs with Tree method for 512 datapoints
Took 20 msecs with Tree method for 1024 datapoints
Took 50 msecs with Tree method for 2048 datapoints
Took 108 msecs with Tree method for 4096 datapoints
Took 194 msecs with Tree method for 8192 datapoints
Took 396 msecs with Tree method for 16384 datapoints
Took 837 msecs with Tree method for 32768 datapoints
Took 1741 msecs with Tree method for 65536 datapoints
Took 3596 msecs with Tree method for 131072 datapoints
```

```
Took 7824 msecs with Tree method for 262144 datapoints
Took 18207 msecs with Tree method for 524288 datapoints
Took 40017 msecs with Tree method for 1048576 datapoints
```



We can see, algorithm is scaling well with data-set size n. If we analyse the complexity of algorithm, its linearithmin , i.e. $\Theta(n \log n)$.

In [228]: