Validation

December 7, 2020

[ ]:
```
![ -e 'zip.train' ] || ( wget https://web.stanford.edu/~hastie/ElemStatLearn/
↪datasets/zip.train.gz && gzip -d zip.train.gz )
![ -e 'zip.test' ] || ( wget https://web.stanford.edu/~hastie/ElemStatLearn/
↪datasets/zip.test.gz && gzip -d zip.test.gz )
```

Import necessary packages: Numpy, Pandas, matplotlib

[ ]:
```
import numpy as np
import pandas as pd
from matplotlib import pyplot as plt
```

Mount your google drive (if you have a google account) or upload files (go on the file icon on the left -> right click). Copy path of zip.train and zip.test and load them as numpy arrays using the following code (insert the path as string).

[ ]:
```
#dirname = '/content/drive/My Drive/ML_Class_2020/KNN/'
dirname = './'
path_to_train = dirname + 'zip.train'
path_to_test = dirname + 'zip.test'
training_data = np.array(pd.read_csv(path_to_train, sep=' ', header=None))
test_data = np.array(pd.read_csv(path_to_test, sep =' ',header=None))

X_train, y_train = training_data[:,1:-1], training_data[:,0]
X_test, y_test = test_data[:,1:], test_data[:,0]

# We only want to classify two different digits. Note the only difference is
# that we don't load as many ones as we load zeros.

X_train_0 = X_train[y_train == 0]
X_train_1 = X_train[y_train == 1][:30]
X_train = np.vstack((X_train_0, X_train_1))

y_train_0 = y_train[y_train == 0]
y_train_1 = y_train[y_train == 1][:30]
y_train = np.hstack((y_train_0, y_train_1))

X_test_0 = X_test[y_test == 0]
X_test_1 = X_test[y_test == 1][:12]
```

```
X_test = np.vstack((X_test_0, X_test_1))

y_test_0 = y_test[y_test == 0]
y_test_1 = y_test[y_test == 1][:12]
y_test = np.hstack((y_test_0, y_test_1))
print(y_test.shape)
```

(371,)

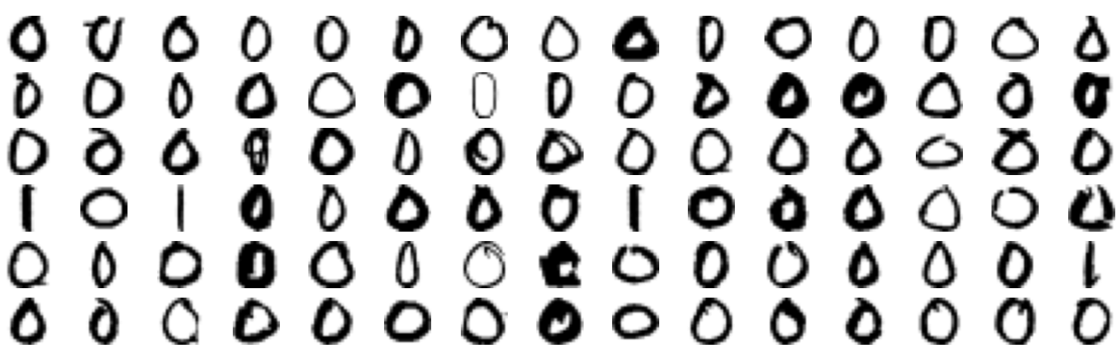
[ ]:
```
def show_numbers(X):
    num_samples = 90
    indices = np.random.choice(range(len(X)), num_samples)
    print(indices.shape)
    sample_digits = X[indices]

    fig = plt.figure(figsize=(20, 6))

    for i in range(num_samples):
        ax = plt.subplot(6, 15, i + 1)
        img = 1-sample_digits[i].reshape((16, 16))
        plt.imshow(img, cmap='gray')
        plt.axis('off')
```

[ ]:
```
show_numbers(X_test)
```

(90,)



Choose one of the classifiers you implemented and use it on the following task: Take a look at the provided notebook. It loads the ZIP-Code's zeros and ones, but now there are manymore zeros than there are ones. We are going to believe that these digits represent geneticdata. Actually, we are virologists trying to develop a test to determine which of the data belongs to infected patients (the ones) and which do not (the zeros). Train/apply your model on the data and do the tasks of the exercise.

[ ]:

```python
from collections import Counter
from functools import wraps, partial


def collect_after(c):
  def decorator(f):
    @wraps(f)
    def g(*args, **kwargs):
      return c(f(*args, **kwargs))
    return g
  return decorator


class KNearestNeighbors():
    '''
    Think about defining more functions that will help you building this␣
 ↪algorithm.
    Optimally, one that takes in k and a test image as a parameter.
    '''
    def squared_euclidean_distance(self, x_1, x_2, axis=1):
      '''
      np.sum(x, axis = 1) will be summing all elements over the pixel dimension␣
 ↪(axis = 1)
      '''
      return np.sum((x_1 - x_2) ** 2, axis=axis)

    def set_k(self, k):
      self.k = k

    def __init__(self, k):
      self.set_k(k)

    def fit(self, X, y):
      self.X = X
      self.y = y

    @collect_after(tuple)
    def calculate_nearest(self, X, k=None):
      if k is None:
        k = self.k
      for obj in X:
        nearest = []
        for i, known in enumerate(self.X):
          d = self.squared_euclidean_distance(known, obj, axis=0)
          nearest.append((d, i))
          nearest.sort()
          nearest[k:] = []
```

```
        yield tuple(nearest)

    @collect_after(partial(np.fromiter, dtype=float))
    def predict_class(self, X, nearest=None):
      res = []
      k = self.k
      if nearest is None:
        nearest = self.calculate_nearest(X, k)
      for nearest_current in nearest:
        yield Counter(self.y[i] for _, i in nearest_current[:k]).
↪most_common(1)[0][0]

    def predict_class_different_k(self, X, ks=(3,)):
      ks = tuple(ks)
      nearest = self.calculate_nearest(X, max(ks))
      for k in ks:
        self.set_k(k)
        yield (k, self.predict_class(X, nearest=nearest))


def accuracy(y_actual, y_pred):
  return (y_actual == y_pred).sum() / len(y_actual)
```

[ ]:
```
@collect_after(tuple)
def k_fold_split(X, y, k):
  n = len(y)
  permut = np.argsort(np.random.random_sample((n,)))
  X_s = X[permut]
  y_s = y[permut]
  for i in range(k):
    start, end = int(i * n / k), int((i + 1) * n / k)
    yield (X_s[start:end], y_s[start:end])
```

[ ]:
```
class CrossValidation():
  def stack_pairs(self, pairs):
    return np.vstack([Xy[0] for Xy in pairs]), np.hstack([Xy[1] for Xy in␣
↪pairs])

  def joins(self, samples):
    for i in range(len(samples)):
      yield (samples[i], self.stack_pairs(samples[:i] + samples[i + 1:]))

  def __init__(self, model_class, samples, params, loss):
    self.models = []
    self.train_val_splits = []
    losses = []
    for Xy_val, Xy_train in self.joins(samples):
```

```python
            self.train_val_splits.append((Xy_train, Xy_val))
            model = model_class(**params)
            self.models.append(model)
            model.fit(*Xy_train)
            y_pred = model.predict_class(Xy_val[0])
            L = loss(Xy_val[1], y_pred)
            losses.append(L)
        self.losses = np.array(losses)
        self.bias = np.mean(self.losses)
        self.var = np.var(self.losses)
```

[ ]:
```python
def one_minus_accuracy(y_actual, y_pred):
  return 1.0 - accuracy(y_actual, y_pred)
```

[ ]:
```python
from itertools import product
def iter_params(spaces):
  names = spaces.keys()
  for values in product(*(spaces[k] for k in names)):
    yield dict(zip(names, values))
```

[ ]:
```python
def k_fold_search_params(model_class, X, y, k, spaces, loss):
  info = {**{'param_' + i: [] for i in spaces.keys()}, 'bias': [], 'var': []}
  splits = k_fold_split(X, y, k)
  for params in iter_params(spaces):
    cv = CrossValidation(model_class, splits, params, loss)
    info['bias'].append(cv.bias)
    info['var'].append(cv.var)
    for p, v in params.items():
      info['param_' + p].append(v)
  return pd.DataFrame(info)
```

[ ]:
```python
%%time
np.random.seed(42)
search_df = k_fold_search_params(KNearestNeighbors, X_train, y_train, 5, {'k':␣
 ↪np.arange(1, 30, 1, dtype=int)}, one_minus_accuracy)
```

```
CPU times: user 5min 6s, sys: 57.8 ms, total: 5min 6s
Wall time: 5min 7s
```

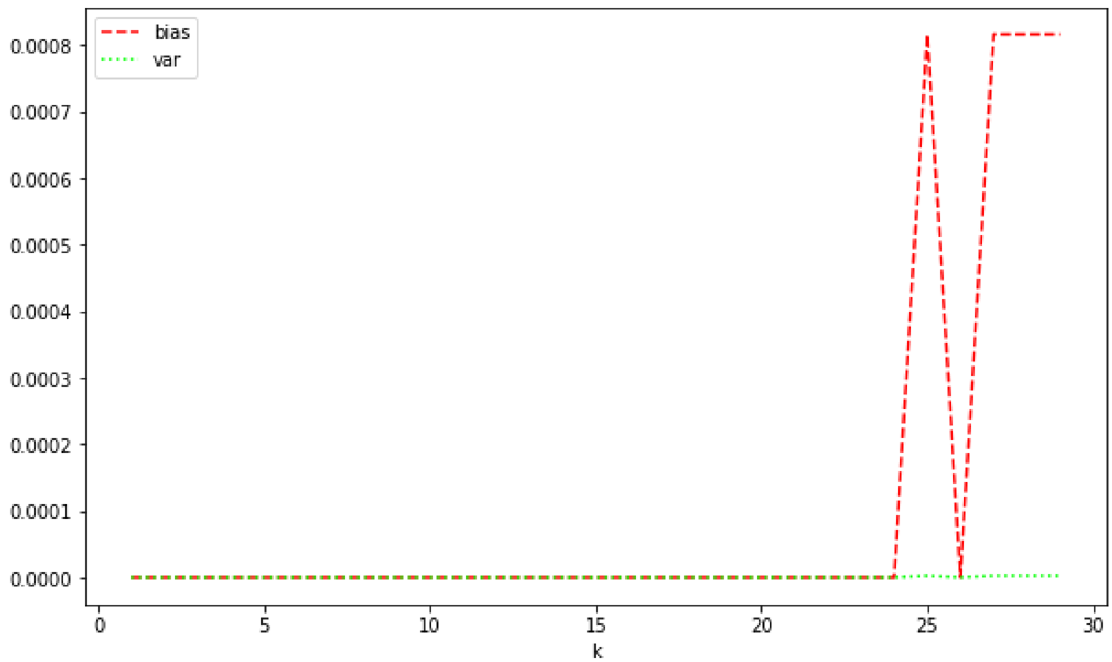
[ ]:
```python
search_df
```

[ ]:

	param_k	bias	var
0	1	0.000000	0.000000
1	2	0.000000	0.000000
2	3	0.000000	0.000000
3	4	0.000000	0.000000
4	5	0.000000	0.000000

```
5           6  0.000000  0.000000
6           7  0.000000  0.000000
7           8  0.000000  0.000000
8           9  0.000000  0.000000
9          10  0.000000  0.000000
10         11  0.000000  0.000000
11         12  0.000000  0.000000
12         13  0.000000  0.000000
13         14  0.000000  0.000000
14         15  0.000000  0.000000
15         16  0.000000  0.000000
16         17  0.000000  0.000000
17         18  0.000000  0.000000
18         19  0.000000  0.000000
19         20  0.000000  0.000000
20         21  0.000000  0.000000
21         22  0.000000  0.000000
22         23  0.000000  0.000000
23         24  0.000000  0.000000
24         25  0.000816  0.000003
25         26  0.000000  0.000000
26         27  0.000816  0.000003
27         28  0.000816  0.000003
28         29  0.000816  0.000003
```

[ ]:
```
plt.figure(figsize=(10, 6))
plt.plot(search_df['param_k'], search_df['bias'], linestyle='--',␣
 ↪color='#FF0000', label='bias')
plt.plot(search_df['param_k'], search_df['var'], linestyle=':',␣
 ↪color='#00FF00', label='var')
plt.xlabel('k')
plt.legend()
plt.show()
```



The model seems to almost always give the correct answer on the training dataset.

[ ]:
```python
from collections import namedtuple
from functools import lru_cache

class Confusion(namedtuple('Confusion', ['TP', 'FP', 'FN', 'TN'])):
  def calculate(y_true, y_pred):
    y_true = y_true == True
    y_pred = y_pred == True
    return Confusion((y_true & y_pred).sum(), (~y_true & y_pred).sum(),
                     (y_true & ~y_pred).sum(), (~y_true & ~y_pred).sum())

  @property
  def P(self):
    return self.TP + self.FN

  @property
  def N(self):
    return self.FP + self.TN

  @property
  def PP(self):
    return self.TP + self.FP

  @property
```

```python
  def PN(self):
    return self.FN + self.TN

  # Precision
  @property
  @lru_cache()
  def PPV(self):
    return self.TP / self.PP

  # Recall
  @property
  @lru_cache()
  def TPR(self):
    return self.TP / self.P

  @property
  def F1(self):
    return 2 / (1 / self.TPR + 1 / self.PPV)

  @property
  def accuracy(self):
    return (self.TP + self.TN) / (self.P + self.N)
```

[ ]:
```python
%%time
model = KNearestNeighbors(k=3)
model.fit(X_train, y_train)
conf = Confusion.calculate(y_test, model.predict_class(X_test))
```

```
CPU times: user 3.6 s, sys: 998 µs, total: 3.6 s
Wall time: 3.6 s
```

[ ]:
```python
conf
```

[ ]:
```
Confusion(TP=12, FP=1, FN=0, TN=358)
```

[ ]:
```python
def print_scores(conf):
  print(f"""
Precision: {conf.PPV:.3}
Recall: {conf.TPR:.3}
F1-score: {conf.F1:.3}
Accuracy: {conf.accuracy:.3}
""")
```

[ ]:
```python
print_scores(conf)
```

```
Precision: 0.923
```

```
Recall: 1.0
F1-score: 0.96
Accuracy: 0.997
```

[ ]:
```
conf_zeros = Confusion.calculate(y_test, np.zeros_like(y_test))
print_scores(conf_zeros)
```

```
Precision: nan
Recall: 0.0
F1-score: nan
Accuracy: 0.968
```

```
/usr/local/lib/python3.6/dist-packages/ipykernel_launcher.py:31: RuntimeWarning:
invalid value encountered in long_scalars
/usr/local/lib/python3.6/dist-packages/ipykernel_launcher.py:41: RuntimeWarning:
divide by zero encountered in double_scalars
```

Precision is not defined, because we have never classified objects as positive, but F1 would be 0 in similar cases.

Precision only says the proportion of correct answers. F1-score shows, how the nodel actually is at distinguishing the two classes.

According to the given test dataset, the probability is 92. Yes, I would.

But even if the probabilities had been less, using the test could be recommended depending on the cost of the two types of error,