sheet04-LaTeX-export

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1 Sheet 4

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1.1 1 Bayes: Signal or Noise?

We know $p(\mathrm{A}|\mathrm{B}) = \frac{p(\mathrm{B}|\mathrm{A})p(\mathrm{A})}{p(\mathrm{B})}$. If we assign A=target direction/not on target, B=gamma/background, we see that:

$$p(\text{gamma ray}|\text{target direction}) = \frac{p(\text{target direction}|\text{gamma ray}) \cdot p(\text{gamma ray})}{p(\text{target direction})} \tag{1}$$

$$= \frac{p(\text{target direction}|\text{gamma ray}) \cdot p(\text{gamma ray})}{p(\text{target direction}|\text{gamma ray}) \cdot p(\text{gamma ray}) + p(\text{target direction}|\text{background}) \cdot p(\text{background})} \tag{2}$$

$$= \frac{0.95 \cdot 0.1}{0.95 \cdot 0.1 + 0.1 \cdot 0.9} = \frac{0.095}{0.095 + 0.09} = \frac{0.095}{0.185} \approx 0.51 = 51\%. \tag{3}$$

1.2 2 Bayes Classifiers

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a) $R(f) = \mathbb{E}_{Y|X=x} L(Y, f(X=x)) = \sum_{y \in \{0,1\}} p(Y=y)^{|X=x} L(Y=y, f(X=x))$

$= p(Y=0|X=x) \cdot 1 \cdot p(f(X) = 1|X=x)$

$+ p(Y=1|X=x) \cdot 10 \cdot p(f(X)=0|X=x)$

is to be minimized. Because $f(x)$ is fixed, we minimize by either setting $f(x)=1$ or $f(x)=0$ $\Rightarrow p(f(x)=1|X=x) = \begin{cases} 0, f(x)=0 \\ 1, f(x)=1 \end{cases}$

Therefore we set: $f(x) = \begin{cases} 1, & \text{if } 10 \cdot p(Y=1|X=x) \geq p(Y=0|X=x) \\ 0 & \text{otherwise} \end{cases}$

Such an asymmetric loss matrix could be used, when one result is highly unfavorable. If we interpret $y \in \{0,1\}$ as false / true, the given matrix would heavily penalize false negatives. This could be used in preliminary medical analyses, where as few as possible diseases may be missed.

b) $R(f) = \mathbb{E}_{Y|X=x} L(Y=y, f(X=x))$

$= \sum_{y \in \{1,\dots,k\} \setminus f(x)} p(Y=y|X=x) \cdot 1$

$+ \alpha \cdot p(f(X)=0|X=x)$

$= 1 - p(f(X)=y|X=x) + \alpha \cdot p(f(X)=0|X=x)$

minimize $\rightarrow$ $f(x) = \begin{cases} \arg\min_y p(y|x), & \text{if } p(y|x) \geq 1-\alpha \\ 0 & \text{otherwise} \end{cases}$

$\rightarrow$ i.e. choose y with highest probability, if it is more probable than $1-\alpha$, otherwise do not decide.

$\rightarrow$ α sets a boundary as to how confident we must be to take a decision. A classifier like this could be used in a 2-step process, where the first step is inexpensive but error-prone and the second process is more costly but accurate. All „0"-results from the 1st step could then be passed on to the second step.

1.3 3 K-Nearest Neighbors: Cross-Validation

[1]:
```
import numpy as np
import matplotlib.pyplot as plt

#bigger plots
plt.rcParams['figure.figsize'] = [12, 8]
plt.rcParams['figure.dpi'] = 300 # higher resolution figures
plt.rc('text', usetex=True) # use LaTeX in axis and plot titles
```

load the data

[2]:
```
# for faster runtimes, we use a subsampled version of the data even as the␣
 ↪'full' dataset
full_features = np.load('data/dijet_features_normalized.npy')[:,::2]#there was␣
 ↪a missing ":," in given code
full_labels = np.load('data/dijet_labels.npy')[::2]

dset_full = (full_features, full_labels)
dset_medium = (full_features[:, ::4], full_labels[::4])
dset_small = (full_features[:, ::16], full_labels[::16])
dsets = (dset_small, dset_medium, dset_full)

for features, labels in dsets:
    print(features.shape, labels.shape, features.dtype, labels.dtype)
```

```
(116, 70) (70,) float64 float64
(116, 280) (280,) float64 float64
(116, 1117) (1117,) float64 float64
```

(a)

[3]:
```
def crossval_splits(features, labels, k):
    """
    compute k-fold cross-validation splits of the features and corresponding␣
 ↪labels

    Parameters
    ----------
    features : np.ndarray
        Feature array of shape (d, N).
    labels : np.ndarray
        Label array of shape (N).
    k : int
        Number of folds.

    Returns
    -------
    list
```

```
        A list of the cross validation splits, i.e. a list splits of length n
        splits[i] = ((training_features_i, training_labels_i), (val_features_i,␣
↪val_labels_i)).

    """
    assert features.shape[-1] == len(labels), f'Shape mismatch: {features.
↪shape}, {labels.shape}'

    # TODO: divide features and labels into (approximately) equal sized chunks
    # Hint: Use np.linspace to get chunk borders and round the results
    split_indices = np.linspace(0,features.shape[-1],k, endpoint=False,␣
↪dtype=int)[1:]
    # np.array_split returns a python list of the split sub-arrays
    featuresplits = np.array_split(features, split_indices, axis=1)
    labelsplits   = np.array_split(labels, split_indices)
    # TODO: Shuffle the data
    # we arrange the data we return in a loop, therefore it is sufficient to␣
↪shuffle the
    # indices over which we loop later
    indices = np.arange(k)
    np.random.shuffle(indices)
    # TODO: Construct a list consisting of the splits; each split consits of
    #       - the validation set (one chunk of the features and corresponding␣
↪labels)
    #       - the training training set (concatenation of all feature and label␣
↪chunks not used for validation)
    # i.e. splits[i] = ((training_features_i, training_labels_i),␣
↪(val_features_i, val_labels_i))
    splits = []
    for i in indices:
        #copy = featuresplits.copy()
        retf = np.empty((full_features.shape[0],0))
        retl = np.empty(0)
        for j in indices:
            if j != i:
                retf = np.append(retf, featuresplits[j],axis=1)
                retl = np.append(retl, labelsplits[j])
        item = [retf, retl,featuresplits[i], labelsplits[i]]
        splits.append(item)
    assert len(splits) == k, f'Got incorrect number of splits: {len(splits)=}!
↪={k=}'
    return splits
```

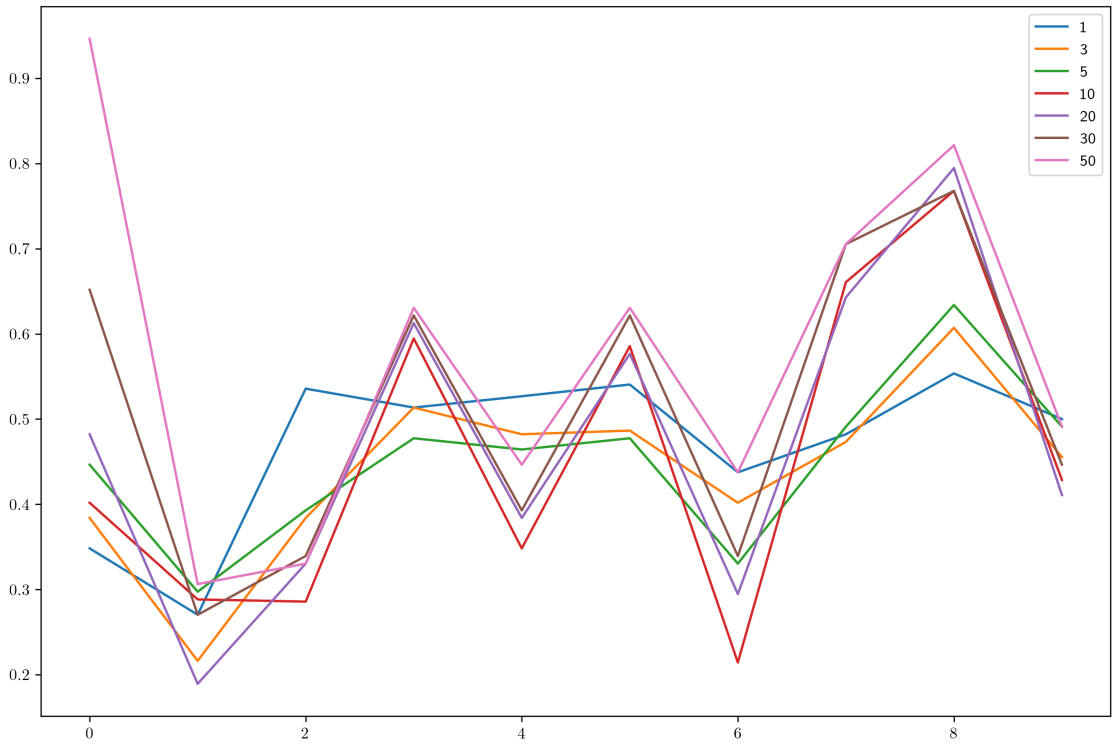
[4]:
```
it = crossval_splits(full_features, full_labels, 5)
print(np.shape(it[0][3]))
```

```
(223,)
```

(b)

[5]:
```
def mean_err(pred, labels):
    """mean error between categorical predictions and labels (each a 1D numpy␣
 ↪array)"""
    # TODO implement this (Hint: compute the mean over a fitting boolean array)
    err = np.mean(np.abs((pred-labels).astype(int)))
    std = np.std(np.abs((pred-labels).astype(int)))
    return err, std
```

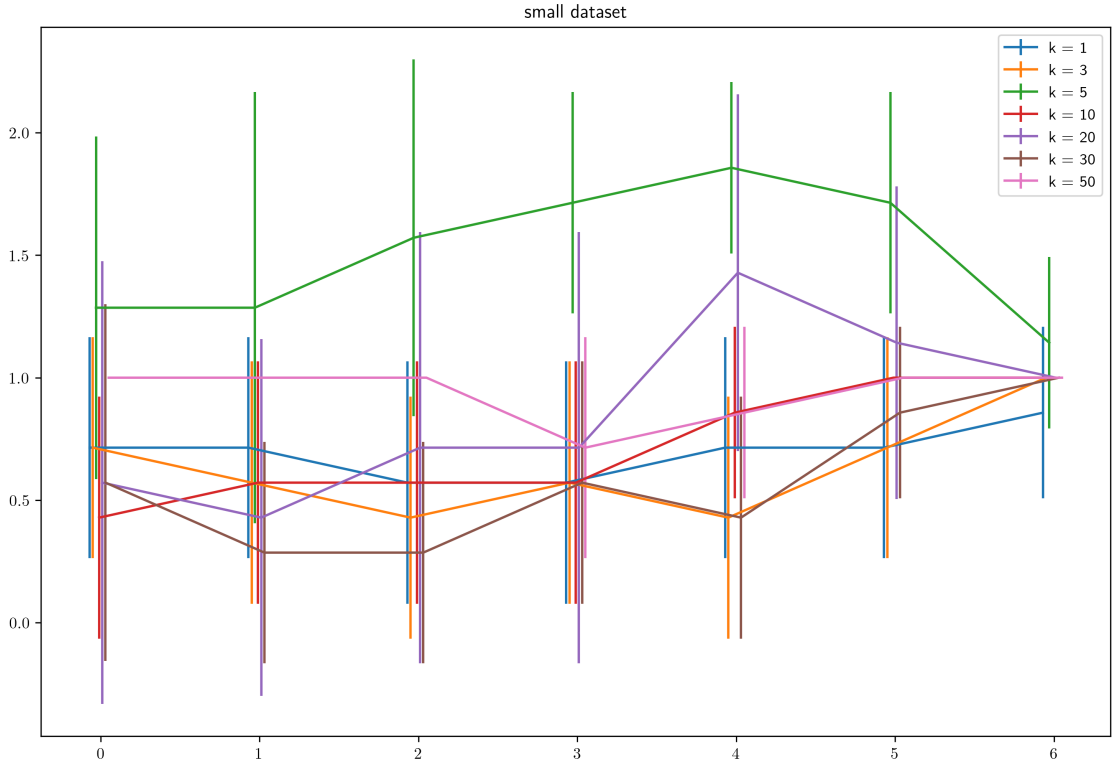
[6]:
```
from sklearn.neighbors import KNeighborsClassifier

ks = (1, 3, 5, 10, 20, 30, 50)
n_folds = 10
errors = np.empty((n_folds, len(ks)))

for i, item in enumerate(crossval_splits(full_features, full_labels, n_folds)):
    train_features, train_labels, val_features, val_labels = item
    for j, k in enumerate(ks):
        # TODO: Use KNeighborsClassifier from sklearn (read the documentation)␣
 ↪to fit the training data and save the validation error
        classif = KNeighborsClassifier(k)
        classif.fit(train_features.T, train_labels)
        errors[i, j], _ =  mean_err(classif.predict(val_features.T), val_labels)


plt.plot(errors,label=['1','3','5','10','20','30','50'])
plt.legend(loc='best')
plt.show()
```

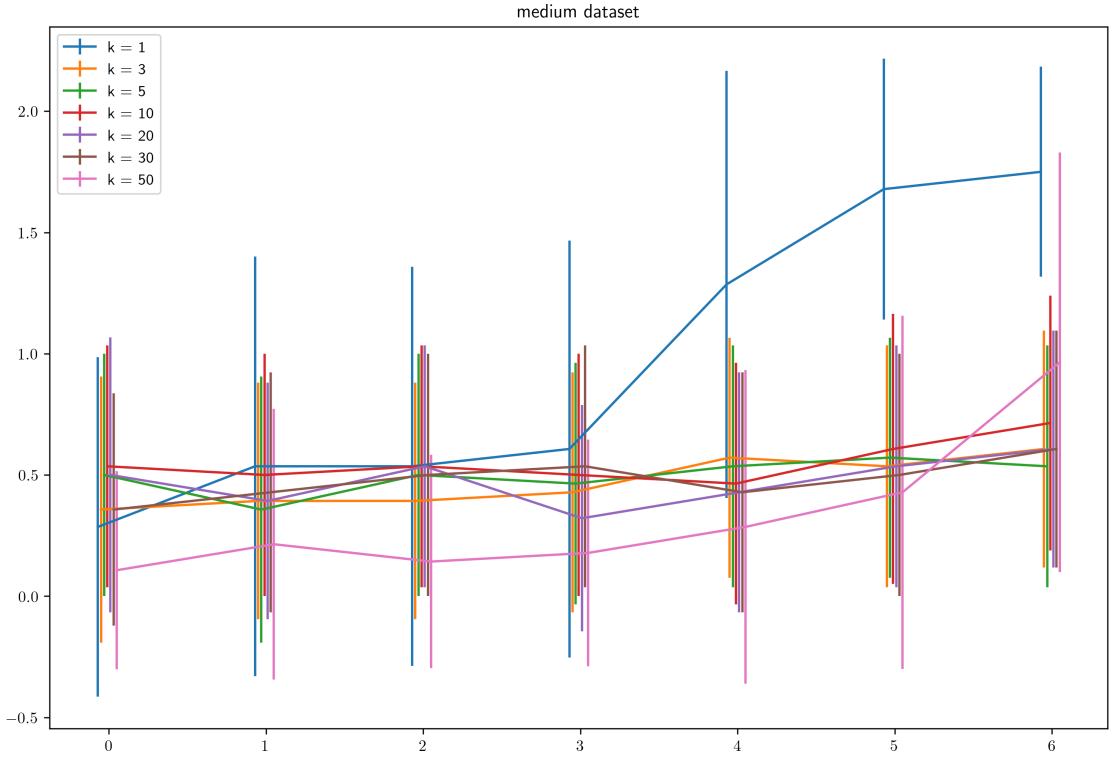


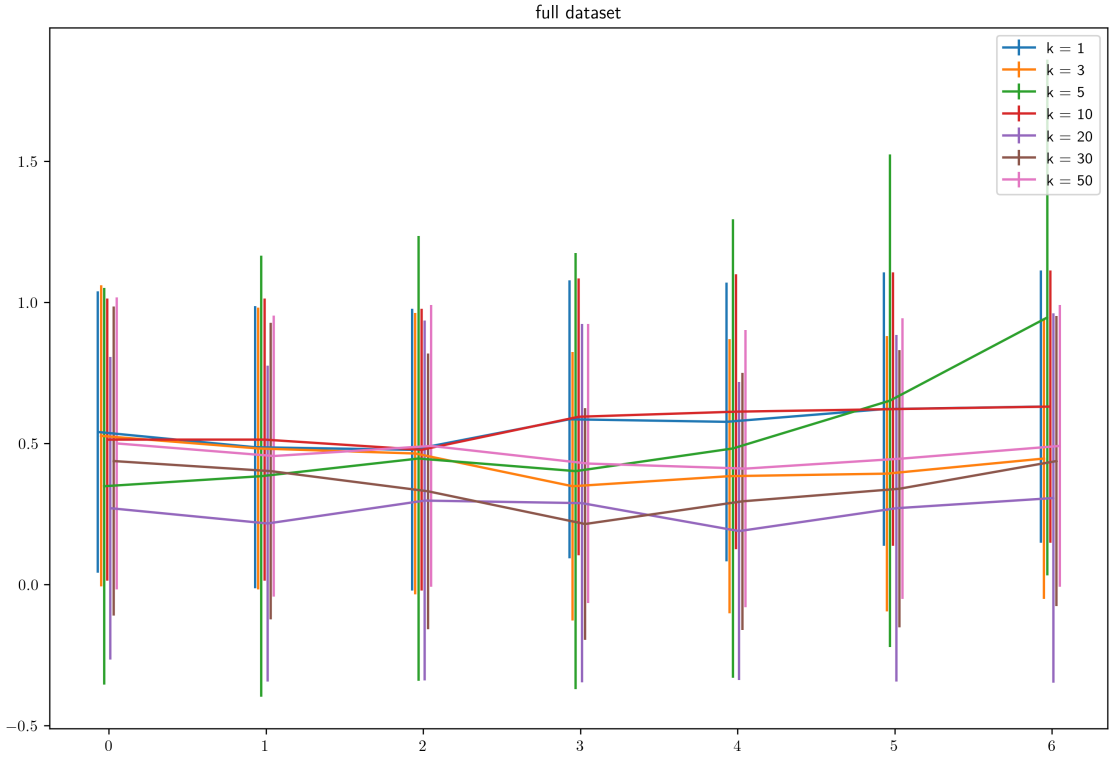
(c)

[7]:
```
from sklearn.neighbors import KNeighborsClassifier

ks = (1, 3, 5, 10, 20, 30, 50)
n_folds = 10
errors = np.empty((len(dsets), n_folds, len(ks)))
stddevs = np.empty((len(dsets), n_folds, len(ks)))

for i, (features, labels) in enumerate(dsets):
    for j, item in enumerate(crossval_splits(features, labels, n_folds)):
        train_features, train_labels, val_features, val_labels = item
        for l, k in enumerate(ks):
            # TODO: Use KNeighborsClassifier from sklearn (read the␣
 ↪documentation) to fit the training data and save the validation error
            classif = KNeighborsClassifier(k)
            classif.fit(train_features.T, train_labels)
            errors[i, j, l], stddevs[i, j, l] =  mean_err(classif.
 ↪predict(val_features.T), val_labels)

for i in range(3):
    for j in range(errors.shape[-1]):
```

```
        xoffs = (j-errors.shape[-1]/2)*0.02 #x-offset to be able to see␣
↪different error bars
        plt.errorbar(np.arange(errors.shape[-1])+xoffs, errors[i,j],␣
↪yerr=stddevs[i,j],
                     label=f'k = {ks[j]}')
    plt.title(['small', 'medium', 'full'][i] + ' dataset')
    plt.legend(loc='best')
    plt.show()
```




medium dataset
k = 1
k = 3
k = 5
k = 10
k = 20
k = 30
k = 50
2.0
1.5
1.0
0.5
0.0
−0.5
0
1
2
3
4
5
6


full dataset
k = 1
k = 3
k = 5
k = 10
k = 20
k = 30
k = 50
1.5
1.0
0.5
0.0
−0.5
0
1
2
3
4
5
6

1.4 4 Alternative K-Nearest Neighbors

1.4.1 a) Relation of laid-out procedure to k-NN classification

For $k = 1$, the procedure is the same as 1-NN classification. For higher values of k, the predicted classes may differ, if the k-th nearest neighbor of the class which has the minority of points in the set of the k-nearest neighbors is closer to the query point than the k-th nearest neighbor of the other class. ### b) More than two classes The algorithm easily generalizes:

(i) Find the k-th nearest neighbor of the query point for each of the other classes.

(ii) Predict that class whose k-th nearest neighbor is closer to the query.

For k=1, this is again the same as the 1-NN classification. For $k \geq 1$, the prediction may differ from that of k-NN again as explained above. The relation thus stays the same.