

## *Solutions 12*

### *Jumping Rivers*

#### *Alternative Dimension Reduction*

We will use the same data set as the previous example so that we can compare the results

```
from sklearn.datasets import make_regression
```

```
X, y, ground_truth = make_regression(  
    n_samples=1000, n_features=1000,  
    n_informative=100, effective_rank=20,  
    random_state=2019, noise=0.2, coef=True  
)
```

a) Create a pipeline for fitting a PCR

```
from sklearn.decomposition import PCA  
from sklearn.pipeline import Pipeline  
from sklearn.preprocessing import StandardScaler  
from sklearn.linear_model import LinearRegression  
from sklearn.model_selection import GridSearchCV  
from sklearn.metrics import mean_squared_error, make_scorer  
import numpy as np
```

```
pca_pipe = Pipeline([  
    ('preprocess', StandardScaler()),  
    ('pca', PCA()),  
    ('regression', LinearRegression())  
])
```

```
pca_pipe.fit(X,y)
```

```
## Pipeline(memory=None,  
##         steps=[('preprocess',  
##               StandardScaler(copy=True, with_mean=True, with_std=True)),  
##               ('pca',  
##               PCA(copy=True, iterated_power='auto', n_components=None,  
##                   random_state=None, svd_solver='auto', tol=0.0,  
##                   whiten=False)),  
##               ('regression',  
##               LinearRegression(copy_X=True, fit_intercept=True, n_jobs=None,  
##                               normalize=False))],  
##         verbose=False)
```

- b) Use a grid search cross validation to find the optimal number of components to use.

```
params = {
    'pca__n_components': np.arange(1,100)
}
search = GridSearchCV(
    pca_pipe, params, cv=10,
    scoring=make_scorer(mean_squared_error, greater_is_better=False),
    return_train_score=False
)
results = search.fit(X, y)
results.best_score_

## -3.5957437806800945

results.best_params_

## {'pca__n_components': 98}
```

- c) From your GridSearchCV object you can retrieve the best estimator as the `.best_estimator_` attribute. Use this to get a cross validation estimate of the mean squared error for this model.

```
from sklearn.model_selection import cross_validate
from sklearn.metrics import mean_squared_error, make_scorer

score_fn = make_scorer(mean_squared_error)

pcc_model = cross_validate(
    search.best_estimator_, X, y,
    scoring=score_fn, cv=10,
    return_train_score=False
)

pcc_model['test_score'].mean()

## 3.685193649865466
```

- d) How does this compare to the linear model from the previous practical

```
print("""
It looks like performance is worse in this instance
""")

##
## It looks like performance is worse in this instance
```

e) Why do you think this is?

```
print("""
In the training data, the input variables all have similar variation.
PCR finds components while ignoring the response variable
So we struggle here because only a few of the inputs are important, but the
principal component decomposition has no way of knowing this.
Performance gets worse because we are reducing the dimension, throwing away information,
but are not picking out the important variables.
""")

##
## In the training data, the input variables all have similar variation.
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## So we struggle here because only a few of the inputs are important, but the
## principal component decomposition has no way of knowing this.
## Performance gets worse because we are reducing the dimension, throwing away information,
## but are not picking out the important variables.
```

f) Fit a PLS regression and compare

```
from sklearn.cross_decomposition import PLSRegression

pls_pipe = Pipeline([
    ('preprocess', StandardScaler()),
    ('pls', PLSRegression())
])

pls_pipe.fit(X,y)

## Pipeline(memory=None,
##          steps=[('preprocess',
##                  StandardScaler(copy=True, with_mean=True, with_std=True)),
##                ('pls',
##                  PLSRegression(copy=True, max_iter=500, n_components=2,
##                                scale=True, tol=1e-06))],
##          verbose=False)

params = {
    'pls__n_components': np.arange(1,100)
}

search = GridSearchCV(
    pls_pipe, params, cv=10,
    scoring=make_scorer(mean_squared_error, greater_is_better=False),
    return_train_score=False
)
```

```

results = search.fit(X, y)
results.best_score_

## -0.2090607549638625

results.best_params_

## {'pls__n_components': 58}

pls_model = cross_validate(
    search.best_estimator_, X, y,
    scoring=score_fn, cv=10,
    return_train_score=False
)

pls_model['test_score'].mean()

## 0.2090607549638625

print("""
Performance is better than PCR since we now consider the response when
choosing the components. We are still not seeing great improvement over linear regression
because we are including useless parameters.
""")

##
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## choosing the components. We are still not seeing great improvement over linear regression
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```

### *Diagnosing progression of diabetes*

Here we will put together all of the elements we have seen so far to build a model for predicting the progression of diabetes in patients. The data is available as part of the sklearn package.

```

from sklearn.datasets import load_diabetes
import pandas as pd

diabetes = load_diabetes()
X = diabetes.data
y = diabetes.target
feature_names = diabetes.feature_names

full_df = pd.DataFrame(X, columns=feature_names)
full_df['target'] = y

```

- a) Start by producing some exploratory graphics and summary statistics. As a hint for producing plots quickly, you can use the **seaborn** library `pairplot()` function.
- b) Given what we have discussed I want you to tell me about the diabetes data. What interesting things are there? What are important predictors in disease progression. What is the best model you can come up with for predicting disease progression for a new patient.