homework11-skel

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SECTION: 995

CS 5970: Machine Learning Practices

1 Homework 11: Dimensionality Reduction

1.1 Assignment Overview

Follow the TODOs and read through and understand any provided code.

For all plots, make sure all necessary axes and curves are clearly and accurately labeled. Include figure/plot titles appropriately as well.

1.1.1 Task

For this assignment you will be exploring dimensionality reduction using Prinicipal Component Analysis (PCA). Having a large number of features can dramatically increase training times and the likelihood of overfitting. Additionally, it's difficult to visualize and understand patterns in high dimensional spaces. It's not uncommon that a lower dimensional subspace of the full feature space will better characterize trends within the data. PCA is one such technique that attempts to locate such subspaces and projects the data into the determined subspace.

1.1.2 Data set

The BMI data will be utilized. Recall:

- * MI files contain data with the number of action potentials (spikes) for 48 neurons, at multiple time points, for a single fold. There are 20 folds (20 files), where each fold consists of over 1000 times points (the rows). At each time point, we record the number of activations for each neuron for 20 bins. Therefore, each time point has 48 * 20 = 960 columns.
- * theta files record the angular position of the shoulder (in column 0) and the elbow (in column 1) for each time point.
- * dtheta files record the angular velocity of the shoulder (in column 0) and the elbow (in column 1) for each time point.
- * torque files record the torque of the shoulder (in column 0) and the elbow (in column 1) for each time point.
- * time files record the actual time stamp of each time point.

1.1.3 Objectives

• Dimensionality Reduction

• Principal Component Analysis (PCA)

1.1.4 General References

- Guide to Jupyter
- Python Built-in Functions
- Python Data Structures
- Numpy Reference
- Numpy Cheat Sheet
- Summary of matplotlib
- DataCamp: Matplotlib
- Pandas DataFrames
- Sci-kit Learn Linear Models
- Sci-kit Learn Ensemble Models
- Sci-kit Learn Metrics
- Sci-kit Learn Model Selection
- Sci-kit Learn Pipelines
- Sci-kit Learn Preprocessing
- SciPy Paired t-test for Dependent Samples

1.1.5 Hand-In Procedure

- Execute all cells so they are showing correct results
- Notebook:
 - Submit this file (.ipynb) to the Canvas HW11 dropbox
- PDF:
 - File/Print/Print to file -> Produces a copy of the notebook in PDF format
 - Submit the PDF file to the Gradescope HW11 dropbox

```
from mpl_toolkits.mplot3d import Axes3D
     from sklearn.pipeline import Pipeline
     from sklearn.base import BaseEstimator, TransformerMixin
     from sklearn.preprocessing import StandardScaler, PolynomialFeatures
     from sklearn.model_selection import cross_val_score, cross_val_predict
     from sklearn.model_selection import train_test_split, GridSearchCV
     from sklearn.metrics import explained_variance_score, confusion_matrix
     from sklearn.metrics import mean_squared_error, roc_curve, auc, f1_score
     from sklearn.linear model import LinearRegression, SGDClassifier
     from sklearn.linear_model import Ridge, Lasso, ElasticNet
     from sklearn.decomposition import PCA
     import joblib
     FIGWIDTH = 5
     FIGHEIGHT = 5
     FONTSIZE = 10
     plt.rcParams['figure.figsize'] = (FIGWIDTH, FIGHEIGHT)
     plt.rcParams['font.size'] = FONTSIZE
     plt.rcParams['xtick.labelsize'] = FONTSIZE
     plt.rcParams['ytick.labelsize'] = FONTSIZE
     %matplotlib inline
     #https://matplotlib.org/3.1.1/tutorials/introductory/images.html
     plt.style.use('ggplot')
[2]: """ PROVIDED
     Display current working directory of this notebook. If you are using
     relative paths for your data, then it needs to be relative to the CWD.
```

[2]: PosixPath('/home/nigel/Desktop/mlp/homework11')

HOME_DIR = pathlib.Path.home()

2 LOAD DATA

pathlib.Path.cwd()

```
# The set of files in the directory

files = fnmatch.filter(os.listdir(directory), filebase)

files.sort()

# Create a list of Pandas objects; each from a file in the directory that

matches filebase

lst = [pd.read_csv(directory + "/" + file, delim_whitespace=True,

header=None).values for file in files]

# Concatenate the Pandas objects together. ignore_index is critical here

so that

# the duplicate row indices are addressed

return lst
```

```
Load the BMI data from all the folds
From the MI_folds we will predict torque_folds
"""

# may need to adjust file path if you are not working on oscer
dir_name = '/home/nigel/Desktop/mlp/mlp_2020/datasets/bmi/DAT6_08'
MI_folds = read_bmi_file_set(dir_name, 'MI_fold*')
theta_folds = read_bmi_file_set(dir_name, 'theta_fold*')
dtheta_folds = read_bmi_file_set(dir_name, 'dtheta_fold*')
torque_folds = read_bmi_file_set(dir_name, 'torque_fold*')
time_folds = read_bmi_file_set(dir_name, 'torque_fold*')

nfolds = len(MI_folds)
nfolds
```

[4]: 20

```
FOLD 0 (1194, 960) (1194, 2) (1194, 2) (1194, 2) (1194, 1)
FOLD 1 (1105, 960) (1105, 2) (1105, 2) (1105, 2) (1105, 1)
FOLD 2 (1532, 960) (1532, 2) (1532, 2) (1532, 2) (1532, 1)
FOLD 3 (1266, 960) (1266, 2) (1266, 2) (1266, 2) (1266, 1)
FOLD 4 (1499, 960) (1499, 2) (1499, 2) (1499, 2) (1499, 1)
FOLD 5 (1253, 960) (1253, 2) (1253, 2) (1253, 1)
```

```
FOLD 6 (1376, 960) (1376, 2) (1376, 2) (1376, 2) (1376, 1)
    FOLD 7 (1131, 960) (1131, 2) (1131, 2) (1131, 1)
    FOLD 8 (1248, 960) (1248, 2) (1248, 2) (1248, 2) (1248, 1)
    FOLD 9 (1258, 960) (1258, 2) (1258, 2) (1258, 2) (1258, 1)
    FOLD 10 (1266, 960) (1266, 2) (1266, 2) (1266, 2) (1266, 1)
    FOLD 11 (1147, 960) (1147, 2) (1147, 2) (1147, 2) (1147, 1)
    FOLD 12 (1226, 960) (1226, 2) (1226, 2) (1226, 2) (1226, 1)
    FOLD 13 (1239, 960) (1239, 2) (1239, 2) (1239, 2) (1239, 1)
    FOLD 14 (1571, 960) (1571, 2) (1571, 2) (1571, 2) (1571, 1)
            (1360, 960) (1360, 2) (1360, 2) (1360, 2) (1360, 1)
    FOLD 15
    FOLD 16 (1580, 960) (1580, 2) (1580, 2) (1580, 2) (1580, 1)
            (1365, 960) (1365, 2) (1365, 2) (1365, 1)
    FOLD 17
            (1390, 960) (1390, 2) (1390, 2) (1390, 2) (1390, 1)
    FOLD 18
            (1290, 960) (1290, 2) (1290, 2) (1290, 2) (1290, 1)
    FOLD 19
[6]: """ PROVIDED
    Summary statistics
    print("Means")
    all_MI = np.concatenate(MI_folds, axis=0)
    all_theta = np.concatenate(theta_folds, axis=0)
    all dtheta = np.concatenate(dtheta folds, axis=0)
    all_torque = np.concatenate(torque_folds, axis=0)
    all time = np.concatenate(time folds, axis=0)
    df = np.concatenate(([all MI.mean()], np.mean(all_theta, axis=0), np.
     →mean(all_dtheta, axis=0),
                         np.mean(all_torque, axis=0))).reshape(1,-1)
    df = pd.DataFrame(df, columns=['MI', 'Should. angle', 'Elbow angle',
                                    'Should. d_angle', 'Elbow d_angle',
                                    'Should. torque', 'Elbow torque'])
    print(df)
    Means
               Should. angle Elbow angle Should. d_angle Elbow d_angle \
    0 0.52154
                     0.178253
                                  1.617722
                                                  0.011528
                                                                -0.005523
       Should. torque Elbow torque
    0
            -0.000565
                           0.001704
```

3 REGRESSION

From the MI folds we will predict torque folds

```
[7]: """ PROVIDED

Evaluate the training performance of an already trained model
"""
```

```
def compute_rmse(x, y):
    return np.sqrt(np.nanmean((x - y)**2))
def predict_score_rmse(model, X, y):
    Compute the model predictions and cooresponding scores.
    PARAMS:
        X: feature data
        y: corresponding output
    RETURNS:
        rmse: root mean squared error
       score: score computed by the models score() method
        preds: predictions of the model from X
    ,,,
    preds = model.predict(X)
    score = model.score(X, y)
    rmse = compute_rmse(y, preds)
    return rmse, score, preds
def predict_plot(model, X, y, time, titles, xlims=None):
    Compute the model's predicted output
    PARAMS:
       model: already trained model
        X: inputs
        y: outputs
        * For plots
        time: time axis of timestamps
        titles: subplot titles for each output column
        xlims: two element list of the x limits for the plot
    I I I
    # Compute and evaulate predictions on the model
    rmse, score, preds = predict_score_rmse(model, X, y)
    print("RMSE: %.3f" % rmse)
    print("R^2: %.3f" % score)
    noutputs = y.shape[1]
    # Construct the plots
    fig, axs = plt.subplots(noutputs,1, figsize=(25,4))
    fig.subplots_adjust(hspace=.5)
    axs = axs.ravel()
    for i, ax in enumerate(axs):
        ax.plot(time, preds[:,i], 'r', label='Prediction')
        ax.plot(time, y[:,i], 'b', label='True')
        ax.set(title=titles[i], ylabel=r'$\tau$ (N-m)')
        ax.set(xlim=xlims)
```

```
axs[-1].set(xlabel='Time (s)')
axs[0].legend()
```

```
[8]: """ TODO
     Obtain the first 1 folds (i.e. index 0)
     Split the data into X (i.e. the MI_folds) and y (i.e. the torque_folds).
     Hold out a subset of the data, before training and cross validation
     # List of the output column names
     output_names = ['Shoulder', 'Elbow']
     # TODO: Grab the first fold
     Xtrain = MI_folds[0]
     ytrain = torque_folds[0]
     time_trn = time_folds[0]
     # TODO: Obtain 2nd to last fold for validation
     Xval = MI_folds[-2]
     yval = torque_folds[-2]
     time_val = time_folds[-2]
     # TODO: Obtain last fold for testing
     Xtest = MI_folds[-1]
     ytest = torque_folds[-1]
     time_test = time_folds[-1]
     nfeatures = Xtrain.shape[1]
     Xtrain.shape, ytrain.shape, Xval.shape, yval.shape, Xtest.shape, ytest.shape
```

[8]: ((1194, 960), (1194, 2), (1390, 960), (1390, 2), (1290, 960), (1290, 2))

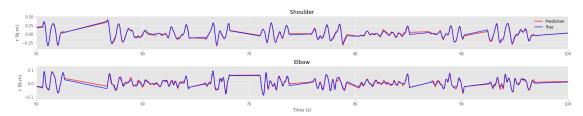
4 BENCHMARK

The task is to predict shoulder and elbow **torque** from the neural activations. We are going to compare the performance of the LinearRegression model trained on the original data to the LinearRegression model trained on the PCA transformed data.

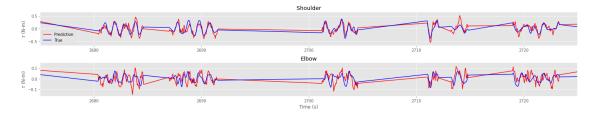
4.1 LinearRegresson Benchmark

```
[9]: """ PROVIDED
LinearRegression benchmark for comparision
"""
benchmark_lnr = LinearRegression()
benchmark_lnr.fit(Xtrain, ytrain)
```

RMSE: 0.017 R^2: 0.959



RMSE: 0.096 R^2: -0.458



5 Principal Component Analysis

```
[11]: """ TODO
    Create a PCA object and fit it on the training set with whiten=True
    """
    model = PCA(whiten=True)
    model.fit(Xtrain, ytrain)
```

[11]: PCA(whiten=True)

[12]: """ TODO

Get an idea of the number of PCs neccessary to represent the data

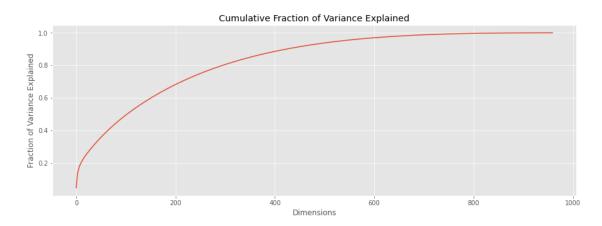
Use pca.explained_variance_ratio to get a fraction for each

```
corresponding PC, and np.cumsum() to get the cumuluative sums as
each component is successively considered.
"""

# TODO: Compute the cumulative fraction of explained variance
explained = model.explained_variance_ratio_.cumsum()

# Plot the cumulative fraction of explained variance
plt.figure(figsize=(FIGWIDTH*3,FIGHEIGHT))
plt.plot(explained)
plt.xlabel('Dimensions')
plt.ylabel('Fraction of Variance Explained')
plt.title('Cumulative Fraction of Variance Explained')
```

[12]: Text(0.5, 1.0, 'Cumulative Fraction of Variance Explained')



```
[13]: """ TODO

Obtain the minimum number of PCs necessary to account for 95% of
the total variance. You can use np.where to locate the indices in
the cumulative sum that is greater than or equal to .95, and then
add 1 to the list of indices returned to get the number of PCs.
The first element in the list is the minimum number of PCs to
account for 95% of the variance.
"""

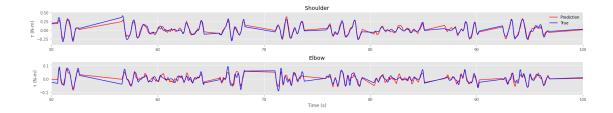
majority_explained = [pc+1 for pc in np.where(explained >= .95)][0]
# Display the determined number of PCs
nPCs = majority_explained[0]
nPCs
```

[13]: 533

[14]: """ TODO
Using the number of PCs obtained above, re-fit the PCA with

```
whiten=True and project the training data into PC space
      pca = PCA(n_components = nPCs, whiten=True)
      pca.fit(Xtrain)
      # TODO: Project into PC-space
      Xtrain_pca = pca.transform(Xtrain)
      Xtrain_pca.shape
[14]: (1194, 533)
[35]: # TODO: Project back into the original space
      Xtrain_recon = pca.inverse_transform(Xtrain_pca)
      Xtrain_recon.shape
[35]: (1194, 960)
[16]: # TODO: Compute the reconstruction error (rmse)
      rmse = compute_rmse(Xtrain, Xtrain_recon)
[17]: """ TODO
      Implement a model Pipeline. The first step of the pipeline is
      PCA with n_components set to the number of PCs determined above
      and whiten to true; and the second step of the pipeline is
      LinearRegression()
      # TODO: Create Pipeline model
      pca_model = Pipeline([
          ('PCA', PCA(n_components = nPCs, whiten=True)),
          ('Regression', LinearRegression())
      ])
      # TODO: Fit model to entire train set
      pca_model.fit(Xtrain,ytrain)
[17]: Pipeline(steps=[('PCA', PCA(n_components=533, whiten=True)),
                      ('Regression', LinearRegression())])
[18]: # TODO: Compute predictions on fully trained model for train set
      # Display the plot of the true output overlaying the predicted output
      # You can use predict_plot() with xlims=[50,100]
      predict_plot(pca_model, Xtrain, ytrain, time_trn,
                   output_names, xlims=[50,100])
     RMSE: 0.031
```

RMSE: 0.031 R^2: 0.868



```
[19]: # TODO: Compute predictions on fully trained model for val set

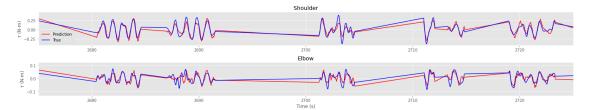
# Display the plot of the true output overlaying the predicted output

# You can use predict_plot() with xlims=[2675,2725]

predict_plot(pca_model, Xval, yval, time_val,

output_names, xlims=[2675,2725])
```

RMSE: 0.053 R^2: 0.616



5.0.1 GRIDSEARCH KFoldHolisticCrossValidation

Use the KFoldHolisticCrossValidation from the HW 11 folder to show training and validation set performance as a function of data set size. The hyper-parameter you should vary for PCA is n_components. Briefly discuss and interepret the results of the GridSearch in terms of train size, performance, and variations in the hyper-parameters.

```
Compute the model predictions and corresponding scores, for an
          already trained model.
          PARAMS:
              model: model to predict with
             X: input feature data
             y: true output for X
             preds: predicted output for X
          RETURNS: results as a dictionary of numpy arrays
             mse: mean squared error for each column
             rmse: rMSE
              evar: explained variance, best is 1.0
             score: score computed by the models score() method
          111
          score = model.score(X, y)
          mse, rmse = mse_rmse(y, preds)
          evar = explained_variance_score(y, preds)
          # Dictionary of numpy arrays. The numpy arrays must
          # be row vectors, where each element is the result
          # for a different output, when using multiple regression.
          # The keys of the dictionary are the name of the performance
          # metric, and the values are the numpy row vectors
          results = {'mse': np.reshape(mse, (1, -1)),
                     'rmse': np.reshape(rmse, (1, -1)),
                     'evar': np.reshape(evar, (1, -1)),
                     'score': np.reshape(score, (1, -1)),
          return results
[21]: # List of number of PCs to try
      components = np.append(np.logspace(0, 5, num=6, base=3, dtype=int), nPCs)
      components
[21]: array([ 1, 3, 9, 27, 81, 243, 533])
[22]: """ TODO
      Create the KFoldHolisticCrossValidation object using the PCA
      pipeline model created above
      Estimated runtime <20 minutes on OSCER
```

Grid Search Parameters

maximize_opt_metric = False
trainsizes = range(1, 11)

opt metric = 'rmse'

rotation_skip = 1

```
# with '__' separated parameter names
      hyperparam_grid = {
          'PCA_n_components': components,
          'PCA_whiten': [True]
      hyperparams = generate_paramsets(hyperparam_grid)
      nhyperparams = len(hyperparams)
      # TODO: Save Parameters. Set these appropriately
      force = False
      write crossval = True
      fullcvfname = "hw11_crossval_%02dparams.pkl" % nhyperparams
      if force or (not os.path.exists(fullcvfname)):
          # TODO: Create the cross validation object. use score eval for the eval func
          crossval = KFoldHolisticCrossValidation(pca_model, hyperparams, score_eval,_
       →opt_metric,
                       maximize opt metric, trainsizes, rotation skip)
          t0 = timelib.time()
          # TODO: Execute cross validation for all parameters and sizes
          crossval.grid_cross_validation(MI_folds, torque_folds)
          # TODO: Save the cross validation object. Can use joblib.dump()
          if write_crossval: joblib.dump(crossval, fullcvfname)
          lapsedTime = timelib.time() - t0
          print(" ** Elapsed Time %.2f min" % (lapsedTime / 60))
      else:
          # TODO: Load the cross val object from file. Can use joblib.load()
          crossval = joblib.load(fullcvfname)
      crossval.model, crossval.rotation_skip, crossval.trainsizes
[22]: (Pipeline(steps=[('PCA', PCA(n_components=533, whiten=True)),
                       ('Regression', LinearRegression())]),
       1,
       range(1, 11))
[23]: """ TODO
      Display the lists of the best parameter sets for each size
      from the cross validation using get_report_best_params_all_sizes
```

TODO: GridSearch pipeline hyper-parameters can be specified

```
display(crossval.get_report_best_params_all_sizes())
```

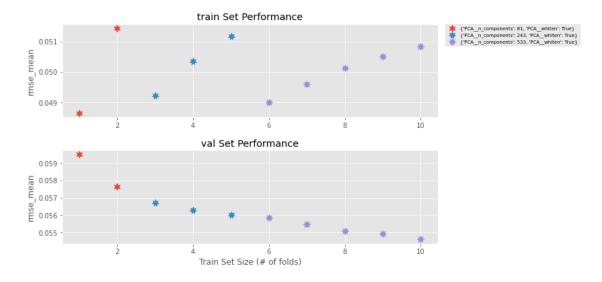
Best Parameter Sets For Each Train Set Size

```
train_size param_index
                                                                paramset
0
                          {'PCA_n_components': 81, 'PCA_whiten': True}
          1
          2
1
                      4
                          {'PCA_n_components': 81, 'PCA_whiten': True}
2
          3
                      5
                        {'PCA_n_components': 243, 'PCA_whiten': True}
3
          4
                        {'PCA_n_components': 243, 'PCA_whiten': True}
4
          5
                        {'PCA_n_components': 243, 'PCA_whiten': True}
5
          6
                        {'PCA_n_components': 533, 'PCA_whiten': True}
                        {'PCA__n_components': 533, 'PCA__whiten': True}
6
          7
7
          8
                         {'PCA_n_components': 533, 'PCA_whiten': True}
8
                         {'PCA_n_components': 533, 'PCA_whiten': True}
          9
9
         10
                      6 {'PCA_n_components': 533, 'PCA_whiten': True}
```

[24]: """ TODO

Plot the mean (summary) train and validation set performances for the best parameter set for each train size for the optimized metrics. Use plot_best_params_by_size()
"""

crossval.plot_best_params_by_size()



```
[25]: """ PROVIDED
        Display available metrics
        crossval.results[0]['results']['val'].keys()
[25]: dict_keys(['mse', 'rmse', 'evar', 'score'])
[26]: """ PROVIDED
        Display available summary (mean and std) metrics
        crossval.results[0]['summary']['val'].keys()
[26]: dict_keys(['mse_mean', 'mse_std', 'rmse_mean', 'rmse_std', 'evar_mean',
        'evar_std', 'score_mean', 'score_std'])
[27]: """ TODO
        Plot the validation results for all parameter sets over all train
        sizes, for the specified metrics, rmse_mean and evar_mean
        (this variable is declared above). Use plot_allparams_val()
        metrics = ['rmse_mean', 'evar_mean']
        crossval.plot_allparams_val(metrics)
[27]: (<Figure size 720x432 with 2 Axes>,
         array([<AxesSubplot:title={'center':'Validation Performance'},</pre>
       ylabel='rmse_mean'>,
                  <AxesSubplot:xlabel='Train Set Size (# of folds)', ylabel='evar_mean'>],
                 dtype=object))
                                         Validation Performance
                                                                                       {'PCA_n_components': 1, 'PCA_whiten': True}
                                                                                       {'PCA_n_components': 3, 'PCA_whiten': True}
{'PCA_n_components': 9, 'PCA_whiten': True}
               0.10
             0.09
0.08
0.07
                                                                                       {PCA_n_components': 27, 'PCA_whiten': True}
{PCA_n_components': 81, 'PCA_whiten': True}
{'PCA_n_components': 243, 'PCA_whiten': True}
{'PCA_n_components': 533, 'PCA_whiten': True}
               0.06
                0.6
              evar_mean
                0.4
                0.2
                0.0
                                                                               10
```

Train Set Size (# of folds)

```
[28]: """ TODO

For the best parameter set for the train set sizes at size_idx=0 (i.e. 1 fold), plot just the TRAIN and VAL set performances using plot_param_train_val() for just the opt_metric
"""

size_idx = 0

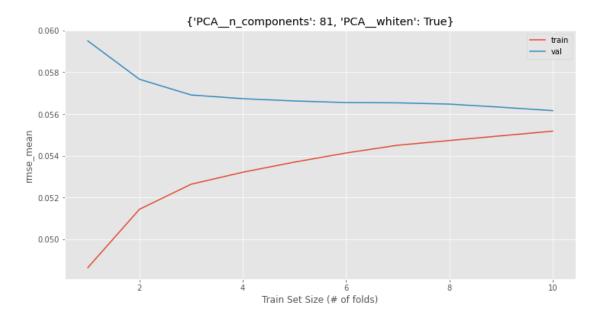
print("Train Set Size", trainsizes[size_idx])

bp_idx = crossval.best_param_inds[size_idx]

# TODO: call plot_param_train_val()

crossval.plot_param_train_val([crossval.opt_metric], bp_idx)
```

Train Set Size 1



```
[29]: """ PROVIDED
Re-fit PCA model with best hyper-parameters for train size of
1 fold
"""
print("Train size %d folds" % trainsizes[0])

bp_idx = crossval.best_param_inds[0]
best_params = crossval.paramsets[bp_idx]

# Set the hyperparameters of the Pipeline model
```

```
pca_model.set_params(**best_params)

# Fit the model to entire train set
pca_model.fit(Xtrain, ytrain)
```

Train size 1 folds

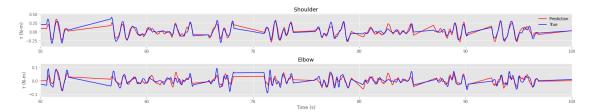
[30]: # TODO: Compute predictions on fully trained model for train set

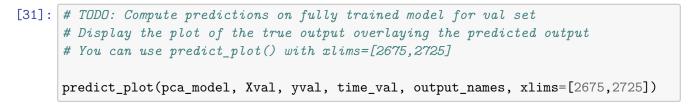
Display the plot of the true output overlaying the predicted output

You can use predict_plot() with xlims=[50,100]

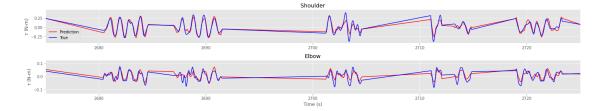
predict_plot(pca_model, Xtrain, ytrain, time_trn, output_names, xlims=[50,100])

RMSE: 0.043 R^2: 0.732





RMSE: 0.049 R^2: 0.640



6 DISCUSSION

1. Bake off. Compare the training and validation performances of the benchmark linear model learned without PCA to the model learned using PCA for train size of 1 fold. Based on the validation performances, which would you choose and why?

I would say that the prediction on the vaidation set performed better with pca. The predictions are closer to the true values without being too perfect for realism, where as the benchmark linear models validation performance was too spikey and not as reliable.

2. Now that you've selected your model, observe and compare the test set results. Was your selection justified? Why or why not?

Yes, because the predictions look more reliable than the linear model.

```
[32]: # TODO: set these paths appropriately

# Re-load saved favorite crossval object

r_crossval = joblib.load('/home/nigel/Desktop/mlp/hw7/hw7_full_ridge_crossval.

→pkl')

# Re-load saved linear crossval object

lnr_crossval = joblib.load('/home/nigel/Desktop/mlp/hw7/

→hw7_full_linear_crossval.pkl')
```

/home/nigel/.local/lib/python3.8/site-packages/sklearn/base.py:329: UserWarning: Trying to unpickle estimator Ridge from version 0.23.1 when using version 0.23.2. This might lead to breaking code or invalid results. Use at your own risk.

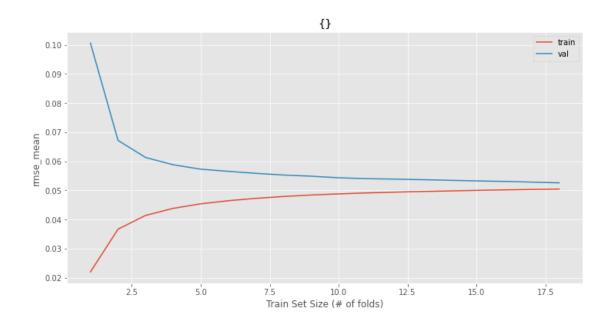
warnings.warn(

/home/nigel/.local/lib/python3.8/site-packages/sklearn/base.py:329: UserWarning: Trying to unpickle estimator LinearRegression from version 0.23.1 when using version 0.23.2. This might lead to breaking code or invalid results. Use at your own risk.

warnings.warn(

```
[33]:

| Display Linear Regression model performance
| """
| lnr_crossval.plot_param_train_val([lnr_crossval.opt_metric])
```



[]: # TODO: any additional plots or tables relevant to your discussion responses