imputing

May 7, 2023

[1]:
```
import pandas as pd
import numpy as np
from scipy import stats

import matplotlib.pyplot as plt
import seaborn as sns
from scipy.interpolate import interp1d
import utils as ut
from sklearn.neighbors import KNeighborsRegressor
from sklearn.model_selection import KFold
from sklearn.model_selection import GridSearchCV

from sklearn.ensemble import VotingRegressor
from sklearn.linear_model import LinearRegression
from sklearn.tree import DecisionTreeRegressor
from sklearn.ensemble import RandomForestRegressor
```

[2]:
```
# CLEANING

# all gene data, includes dpi and gene expression, we only care about the pig␣
↪indexes
gd = pd.read_csv('./allfile_counts.csv', delimiter= '\t', header=0, index_col=0)

# these are normalized values but dont include the pig indices and dpi
gdn = pd.read_csv('./normalized_counts2.txt', delimiter= '\t', header=0,␣
↪index_col=0).transpose()

# give it their respective index, still doesnt have index
gdn.index = gd.index
gdn['dpi'] = gd['dpi']
gdn.head()
```

[2]:
```
       ENSSSCG00000000001  ENSSSCG00000000002  ENSSSCG00000000003
-5001            2.394196           37.110038          790.084684  \
-5001            6.514008           73.825428          837.050071
-5001            3.260678          120.645091          698.600292
-5001            3.593402           72.586721          486.546632
```

```
-5002           5.311616            96.936986           820.644617

       ENSSSCG00000000004  ENSSSCG00000000005  ENSSSCG00000000006
-5001            0.000000          292.091913            2.394196  \
-5001            0.000000          292.044707            1.085668
-5001            0.000000          181.782806            0.000000
-5001            1.437361          102.771297            4.312082
-5002            0.000000          221.317319            0.442635

       ENSSSCG00000000007  ENSSSCG00000000010  ENSSSCG00000000011
-5001          302.865795           14.365176                 0.0  \
-5001          462.494592           20.627693                 0.0
-5001          298.352050           10.597204                 0.0
-5001          237.164533            7.905484                 0.0
-5002          249.203301            5.311616                 0.0

       ENSSSCG00000000013  …  ENSSSCG00000031062  ENSSSCG00000031063
-5001            0.000000  …                 0.0           25.139058  \
-5001            0.000000  …                 0.0           51.026399
-5001            0.000000  …                 0.0           25.270256
-5001            0.000000  …                 0.0           13.654928
-5002            1.327904  …                 0.0           23.017001

       ENSSSCG00000031064  ENSSSCG00000031065  ENSSSCG00000031066
-5001           29.927450                 0.0                 0.0  \
-5001            6.514008                 0.0                 0.0
-5001           10.597204                 0.0                 0.0
-5001            7.905484                 0.0                 0.0
-5002            5.754250                 0.0                 0.0

       ENSSSCG00000031067  ENSSSCG00000031068  ENSSSCG00000031069
-5001                 0.0                 0.0                 0.0  \
-5001                 0.0                 0.0                 0.0
-5001                 0.0                 0.0                 0.0
-5001                 0.0                 0.0                 0.0
-5002                 0.0                 0.0                 0.0

       ENSSSCG00000031070  dpi
-5001                 0.0    0
-5001                 0.0   14
-5001                 0.0   21
-5001                 0.0   28
-5002                 0.0    0

[5 rows x 25323 columns]
```

```
[3]: # only keep columns where the logchange > 0.13, why? idk
     de = pd.read_csv('./deGenes2.txt', delimiter= '\t', header=0, index_col=0)

     # select the genes with logchange > 0.13, idk why
     logchange=0.13
     gdn_keep = gdn[de[de['log2FoldChange'].abs() > logchange].index.tolist()]
     gdn_keep
```

```
[3]:         ENSSSCG00000000574  ENSSSCG00000000915  ENSSSCG00000002471  
     -5001             0.000000           47.883920          426.166890  \
     -5001             0.000000            2.171336         1802.208972   
     -5001             0.815170            3.260678          315.470610   
     -5001             0.000000            2.874722           67.555958   
     -5002             3.983712            6.639520         2194.582532   
     …                        …                   …                   …   
     -5178            26.379492            0.000000         4286.667442   
     -5178             3.918425            5.877637         1180.425389   
     -5186             5.118035          103.640211          594.971580   
     -5186             5.124375            6.405469         1833.245153   
     -5186             0.000000            0.000000          115.783138   

             ENSSSCG00000002780  ENSSSCG00000003140  ENSSSCG00000003497  
     -5001           208.295053            0.000000            0.000000  \
     -5001           113.995146            2.171336            1.085668   
     -5001            89.668649            3.260678            8.966865   
     -5001           310.469934            0.000000            1.437361   
     -5002            20.803828            2.655808            0.885269   
     …                        …                   …                   …   
     -5178            13.189746            1.465527            1.465527   
     -5178            56.817156            1.959212            5.877637   
     -5186            34.546737            2.559018            3.838526   
     -5186            24.340781            1.281094            1.281094   
     -5186            35.862034            3.073889            7.172407   

             ENSSSCG00000006678  ENSSSCG00000007369  ENSSSCG00000009361  
     -5001           134.074977            0.000000           11.970980  \
     -5001           542.834028            0.000000            2.171336   
     -5001           236.399165            0.000000            1.630339   
     -5001           138.705318            0.000000            1.437361   
     -5002           544.440604            0.000000            4.426346   
     …                        …                   …                   …   
     -5178          2041.479572            0.000000            0.000000   
     -5178           518.211644            0.000000            4.898031   
     -5186           586.015019            1.279509           69.093474   
     -5186           810.932342            0.000000           10.248750   
     -5186           131.152582            0.000000            2.049259   
```

```
       ENSSSCG00000010190  ENSSSCG00000010771  ENSSSCG00000011441  
-5001           45.489724            2.394196            1.197098  \
-5001            0.000000            1.085668            0.000000   
-5001            0.000000            0.815170            0.000000   
-5001           11.498886            0.718680            0.000000   
-5002            0.000000            0.000000            0.000000   
…                   …                   …                   …     
-5178            0.000000            0.000000            0.000000   
-5178            0.000000            0.979606            0.000000   
-5186           44.782807            0.000000            0.000000   
-5186            0.000000            0.000000            0.000000   
-5186            0.000000            0.000000            0.000000   

       ENSSSCG00000013311  ENSSSCG00000015717  ENSSSCG00000016157  
-5001            3.591294            0.000000            2.394196  \
-5001            3.257004            0.000000            1.085668   
-5001            2.445509            4.891017            0.000000   
-5001            0.000000            0.000000            0.718680   
-5002            7.967423            0.000000            0.000000   
…                   …                   …                   …     
-5178           20.517383            0.000000            0.000000   
-5178            8.816455            0.979606            0.000000   
-5186            7.677053            0.000000            5.118035   
-5186           16.654219            0.000000            0.000000   
-5186            5.123148            0.000000            0.000000   

       ENSSSCG00000022045  ENSSSCG00000024651  ENSSSCG00000025268  
-5001            0.000000           10.773882           23.941960  \
-5001            2.171336           19.542025            4.342672   
-5001            1.630339           95.374836            4.891017   
-5001            0.000000           41.683463            7.905484   
-5002            0.442635           37.623944            0.885269   
…                   …                   …                   …     
-5178            0.000000           42.500293           17.586328   
-5178            0.000000           32.327002            4.898031   
-5186            0.000000           20.472140           30.708211   
-5186            1.281094            1.281094            1.281094   
-5186            0.000000            8.197036            1.024630   

       ENSSSCG00000025416  ENSSSCG00000026943  
-5001            2.394196            0.000000  
-5001            0.000000            2.171336  
-5001            0.000000            1.630339  
-5001            7.905484            0.718680  
-5002            2.213173            0.442635  
…                   …                   …     
-5178            1.465527           85.000585  
```

```
-5178          5.877637          0.979606
-5186          3.838526          3.838526
-5186          1.281094          2.562187
-5186          1.024630          0.000000

[179 rows x 20 columns]
```

0.1 Testing functions on 1 gene

[4]:
```
# splits dataframe of those with and without na and formats them
w_na, wo_na = ut.na_split('ENSSSCG00000000574', gdn)
```

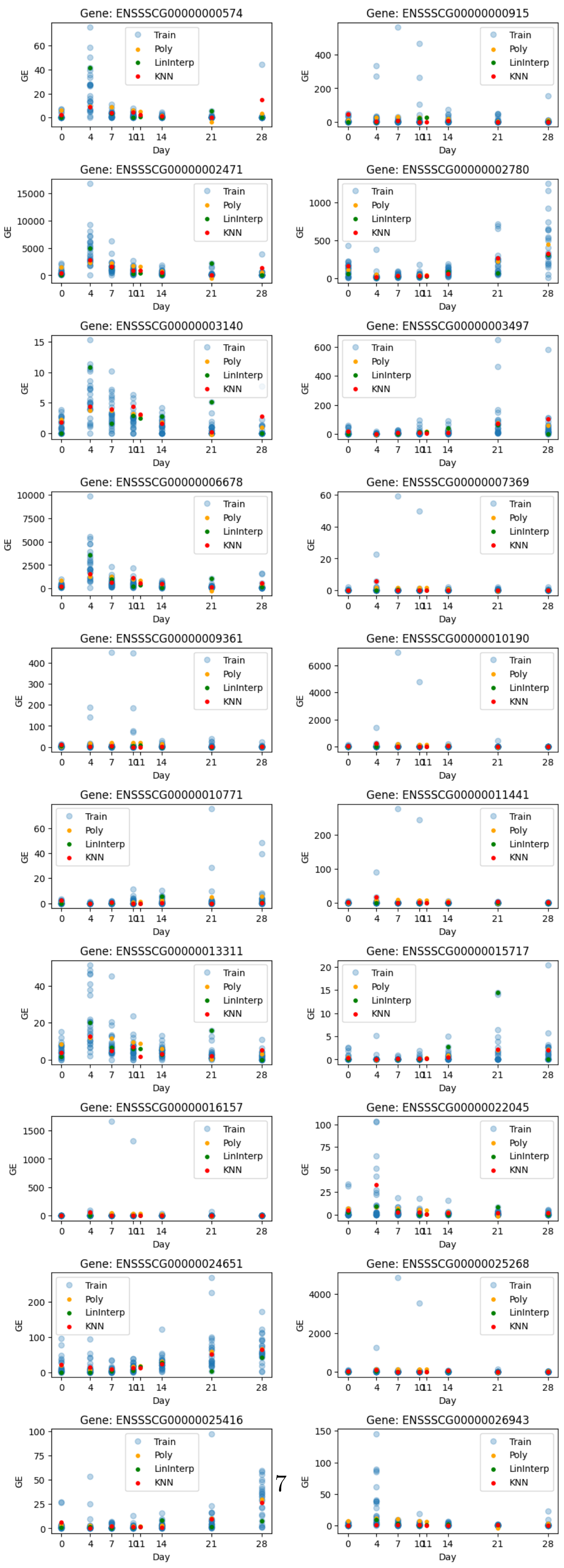
[5]:
```
# performs imputation methods on the split data
poly_df, poly_func, interp_df, interp_func, knn_df, knn_func, knn_scores = ut.
 ↪impute_methods(w_na, wo_na)
```

[6]:
```
knn_scores
```

[6]:
```
93.47172135402197
```

0.2 Plotting the spline and polynomial and knn imputations

[7]:
```
nrows = int(len(gdn_keep.columns)/2)  # number of rows in subplot grid
ncols = 2  # number of columns in subplot grid
fig, axs = plt.subplots(nrows=nrows, ncols=ncols, figsize=(10, 30))

fig.subplots_adjust(hspace=0.5, wspace=0.3)

knn_mses = []
for i, gene in enumerate(gdn_keep.columns):
    row = i // ncols
    col = i % ncols
    ax = axs[row, col]

    w_na, wo_na = ut.na_split(gene, gdn)
    _, poly_func, _, interp_func, _, knn_func, knn_mse = ut.
 ↪impute_methods(w_na, wo_na)
    knn_mses.append(knn_mse)

    # plot scatter plot
    ax.plot(wo_na['day'], wo_na['ge'], 'o', alpha=0.3)

    ##### prediction points
    # these are the actual points we would impute if on the factor levels

    # add scatter plot
    x_points = np.unique(gdn['dpi'])
    interp_y_points = interp_func(x_points)
    poly_y_points = poly_func(x_points)
    knn_y_points = knn_func.predict(x_points.reshape(-1,1)).ravel()

    ax.scatter(x_points, poly_y_points, c='orange', s=15, alpha=1, zorder=10)
    ax.scatter(x_points, interp_y_points, c='green', s=15, alpha=1, zorder=10)
    ax.scatter(x_points, knn_y_points, c='red', s=15, alpha=1, zorder=10)


    # add labels and legend
    ax.set_xlabel('Day')
    ax.set_ylabel('GE')
    ax.legend(['Train', 'Poly', 'LinInterp', 'KNN'])
    ax.set_title(f'Gene: {gene}')
    ax.set_xticks(x_points)


plt.show()
```


Gene: ENSSSCG00000000574
Gene: ENSSSCG00000000915
Gene: ENSSSCG00000002471
Gene: ENSSSCG00000002780
Gene: ENSSSCG00000003140
Gene: ENSSSCG00000003497
Gene: ENSSSCG00000006678
Gene: ENSSSCG00000007369
Gene: ENSSSCG00000009361
Gene: ENSSSCG00000010190
Gene: ENSSSCG00000010771
Gene: ENSSSCG00000011441
Gene: ENSSSCG00000013311
Gene: ENSSSCG00000015717
Gene: ENSSSCG00000016157
Gene: ENSSSCG00000022045
Gene: ENSSSCG00000024651
Gene: ENSSSCG00000025268
Gene: ENSSSCG00000025416
Gene: ENSSSCG00000026943
Train
Poly
LinInterp
KNN
GE
Day

```
[8]: # combine all data
poly_dfs = []
interp_dfs = []
knn_dfs = []

for i, gene in enumerate(gdn_keep.columns):
    # call same methods as before
    w_na, wo_na = ut.na_split(gene, gdn)
    poly_df, poly_func, interp_df, interp_func, knn_df, knn_func, _ = ut.
 ↪impute_methods(w_na, wo_na)

    # create a column of just the gene
    poly_df = poly_df.assign(gene=[gene] * len(poly_df))
    interp_df = interp_df.assign(gene=[gene] * len(interp_df))
    knn_df = knn_df.assign(gene=[gene] * len(knn_df))



    # add values to a list
    poly_dfs.append(poly_df)
    interp_dfs.append(interp_df)
    knn_dfs.append(knn_df)

# combine row bind to create a complete dataframe
poly_df = pd.concat(poly_dfs, axis=0)
interp_df = pd.concat(interp_dfs, axis=0)
knn_df = pd.concat(knn_dfs, axis=0)
```

```
[ ]:
```

Saw some paper that said to calcualte these. nice

https://www.frontiersin.org/articles/10.3389/fgene.2019.00120/full

```
[9]: # group by gene and day, and get the max ge value for each day
df_max = poly_df.groupby(['gene', 'day'])['ge'].max().reset_index().
 ↪rename(columns={'ge':'ge_max'})


# get the max ge value at day 0 for each gene
df_max_day0 = df_max[df_max['day'] == 0].rename(columns={'ge_max': 'ge_day0'})

# merge the two dataframes to get the ge_day0 value for each day and gene
df_merge = pd.merge(df_max, df_max_day0[['gene', 'ge_day0']], on='gene')
```

```
# calculate the distance between the max ge value for each day and the max ge␣
↪value at day 0
df_merge['distance'] = df_merge['ge_max'] - df_merge['ge_day0']

df_merge.head()
```

```
[9]:                  gene  day     ge_max   ge_day0   distance
     0  ENSSSCG00000000574    0   7.069666  7.069666   0.000000
     1  ENSSSCG00000000574    4  75.318073  7.069666  68.248407
     2  ENSSSCG00000000574    7  11.212574  7.069666   4.142908
     3  ENSSSCG00000000574   10   7.525110  7.069666   0.455444
     4  ENSSSCG00000000574   14   4.269556  7.069666  -2.800110
```

```
[10]: # df_merge2 = df_merge.sort_values(['gene','ge_max'])

      # finding the width

      # Subtract the shifted column from the original column
      df_merge['width'] = df_merge['ge_max'] - df_merge.groupby('gene')['ge_max'].
       ↪shift(2)
      df_merge['width'] = df_merge['width'].shift(-1)

      # Fill the first row of each group with 0
      df_merge.loc[df_merge.groupby('gene').head(1).index, 'width'] = 0

      df_merge.head()
```

```
[10]:                  gene  day     ge_max   ge_day0   distance      width
      0  ENSSSCG00000000574    0   7.069666  7.069666   0.000000   0.000000
      1  ENSSSCG00000000574    4  75.318073  7.069666  68.248407   4.142908
      2  ENSSSCG00000000574    7  11.212574  7.069666   4.142908 -67.792963
      3  ENSSSCG00000000574   10   7.525110  7.069666   0.455444  -6.943018
      4  ENSSSCG00000000574   14   4.269556  7.069666  -2.800110  -1.722267
```

```
[11]: # interpolation :) to predict last value

      from scipy.interpolate import CubicSpline
      # Group by gene and sort by day
      df_merge = df_merge.sort_values(by=['gene', 'day'])

      # Interpolate to predict the last value
      width_interpolated = df_merge.groupby('gene')['width'].apply(lambda x: x.
       ↪interpolate(method='index'))
      df_merge['width'] = width_interpolated.reset_index(level=0, drop=True)

      df_merge.head()
```

[11]:
```
                 gene  day     ge_max    ge_day0   distance      width
0  ENSSSCG00000000574    0   7.069666   7.069666   0.000000   0.000000
1  ENSSSCG00000000574    4  75.318073   7.069666  68.248407   4.142908
2  ENSSSCG00000000574    7  11.212574   7.069666   4.142908 -67.792963
3  ENSSSCG00000000574   10   7.525110   7.069666   0.455444  -6.943018
4  ENSSSCG00000000574   14   4.269556   7.069666  -2.800110  -1.722267
```

0.3 Modeling

[12]:
```python
# # get dummies for column gene
# dummies = pd.get_dummies(poly_df['gene'])

# # concatenate dummies with original dataframe
# poly_df2 = pd.concat([poly_df, dummies], axis=1)
```

Modeling to predict the gene expression given the day

[13]:
```python
poly_df2 = poly_df.groupby(['day', 'gene'])['ge'].agg(list).unstack('gene')
poly_df2 = poly_df2.apply(pd.Series.explode).reset_index()
```

[14]:
```python
poly_df2
```

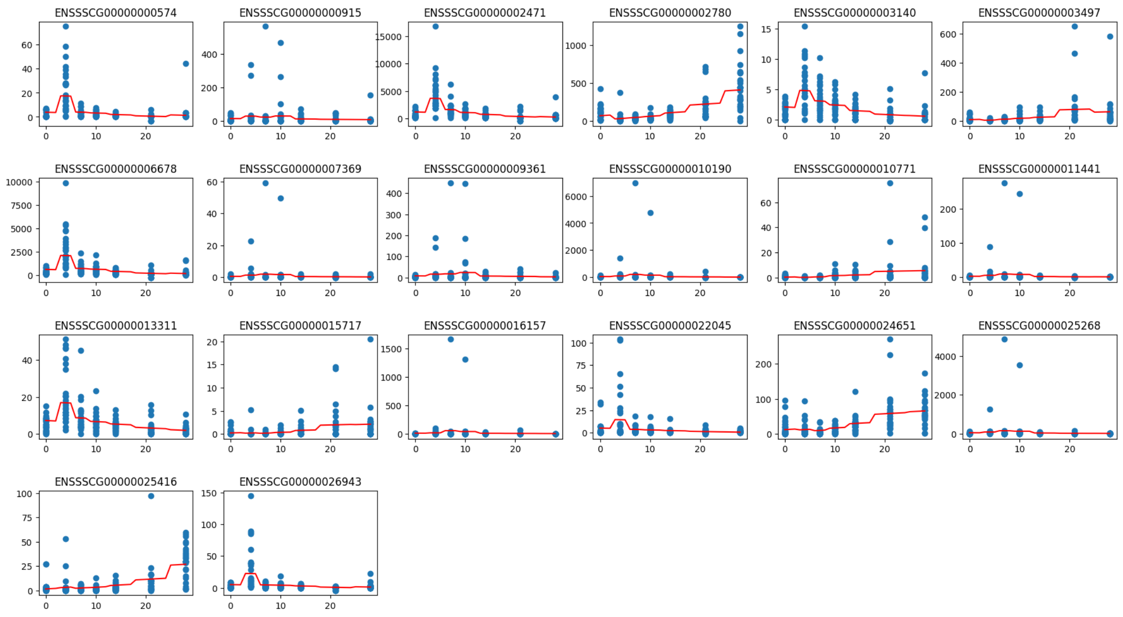
[14]:
```
gene  day ENSSSCG00000000574 ENSSSCG00000000915 ENSSSCG00000002471  \
0       0           6.238112           11.91099         1502.34737
1       0                0.0           3.008567         839.390313
2       0                0.0           1.110826         218.277334
3       0                0.0           6.189792         285.762042
4       0           0.702976           3.514879         355.002736
..    …                  …                  …                  …
191    28           3.283346           9.858927         586.611434
192    28           3.283346           9.858927         586.611434
193    28           3.283346           9.858927         586.611434
194    28                0.0           4.246068           23.77798
195    28                0.0           2.874722          67.555958

gene ENSSSCG00000002780 ENSSSCG00000003140 ENSSSCG00000003497  \
0            107.973612            2.20849          17.412689
1             72.205618                0.0          15.042837
2             61.095437           0.555413           2.777065
3             20.632638                0.0           1.031632
4            170.823099           2.811903           0.702976
..                  …                  …                  …
191          443.226388           0.935961           60.30451
192          443.226388           0.935961           60.30451
193          443.226388           0.935961           60.30451
194          218.247892                0.0          12.738204
195          310.469934                0.0           1.437361
```

```
gene ENSSSCG00000006678 ENSSSCG00000007369 ENSSSCG00000009361  …
0            839.690352           0.170736           3.431027  …  \
1            337.962408                0.0           4.011423  …
2            208.835312           0.555413           3.887891  …
3            143.396837           2.063264                0.0  …
4            342.349173                0.0           3.514879  …
..                  …                  …                 …   …
191          379.155077           0.237516           3.289689  …
192          379.155077           0.237516           3.289689  …
193          379.155077           0.237516           3.289689  …
194           44.159107                0.0           1.698427  …
195          138.705318                0.0           1.437361  …

gene ENSSSCG00000010771 ENSSSCG00000011441 ENSSSCG00000013311
0              0.790758           0.060099           8.488557  \
1              2.005712                0.0           7.019991
2                   0.0                0.0           3.887891
3                   0.0                0.0            5.15816
4                   0.0                0.0           4.217854
..                  …                  …                 …
191            5.501839           0.668844           3.138026
192            5.501839           0.668844           3.138026
193            5.501839           0.668844           3.138026
194            1.698427                0.0           1.698427
195             0.71868                0.0                0.0

gene ENSSSCG00000015717 ENSSSCG00000016157 ENSSSCG00000022045
0              0.513342          -4.928786           7.239431  \
1                   0.0                0.0                0.0
2              0.555413                0.0           3.332478
3                   0.0           1.031632           2.063264
4                   0.0           3.514879           1.405951
..                  …                  …                 …
191            2.137234           1.632316            2.02331
192            2.137234           1.632316            2.02331
193            2.137234           1.632316            2.02331
194            2.547641                0.0                0.0
195                 0.0            0.71868                0.0

gene ENSSSCG00000024651 ENSSSCG00000025268 ENSSSCG00000025416
0             19.894313           5.519435            3.77379  \
1              1.002856           1.002856                0.0
2              2.777065           1.110826           2.221652
3               5.15816          10.316319           1.031632
4              14.76249          14.059514           0.702976
..                  …                  …                 …
```

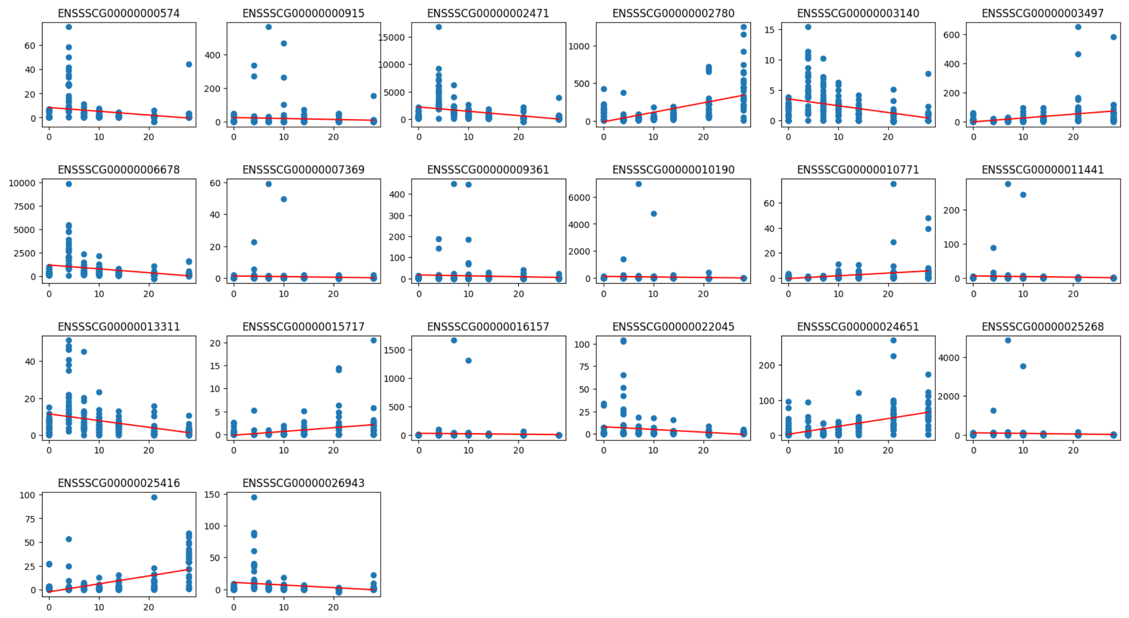
```
191             66.613154           11.417634           29.754741
192             66.613154           11.417634           29.754741
193             66.613154           11.417634           29.754741
194             74.730796            1.698427            21.23034
195             41.683463            7.905484            7.905484

gene ENSSSCG00000026943
0                8.112783
1                5.014279
2                3.332478
3                     0.0
4                0.702976
..                    …
191              3.515169
192              3.515169
193              3.515169
194              0.849214
195               0.71868

[196 rows x 21 columns]
```

[15]:
```python
def regress(df, gene, n):
    # individual models
    model1 = LinearRegression()
    model2 = DecisionTreeRegressor()
    model3 = RandomForestRegressor()

    ensemble_model = VotingRegressor(estimators=[('lr', model1),
                                                 ('dt', model2),
                                                 ('rf', model3)])

    x = df['day'].values.reshape(-1,1)
    y = df[gene].values.reshape(-1,1).ravel()
    ensemble_model.fit(x,y)

    lin = np.arange(0,29).reshape(-1, 1)
    preds = ensemble_model.predict(lin)

    ax = plt.subplot(5, 6, n + 1)
    plt.scatter(df['day'], df[gene])
    plt.plot(lin, preds, color='red')
    plt.title(gene)


plt.figure(figsize=(22, 15))
plt.subplots_adjust(hspace=0.5)
```

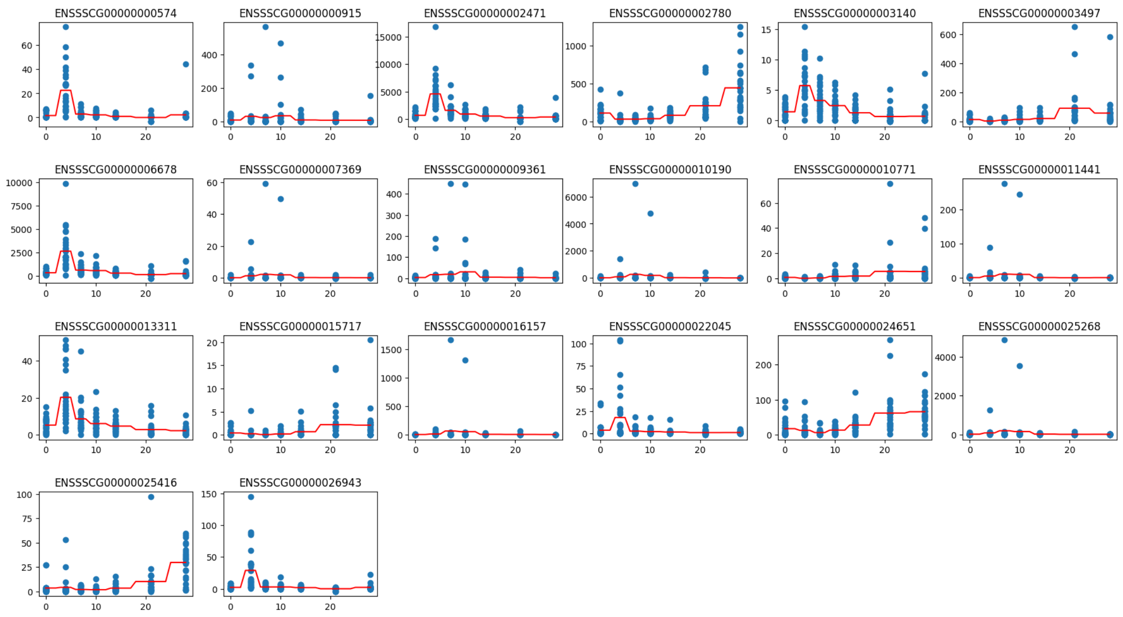
```
for i, gene in enumerate(gdn_keep.columns):

    if gene != 'dpi':

        regress(poly_df2, gene, i)
```



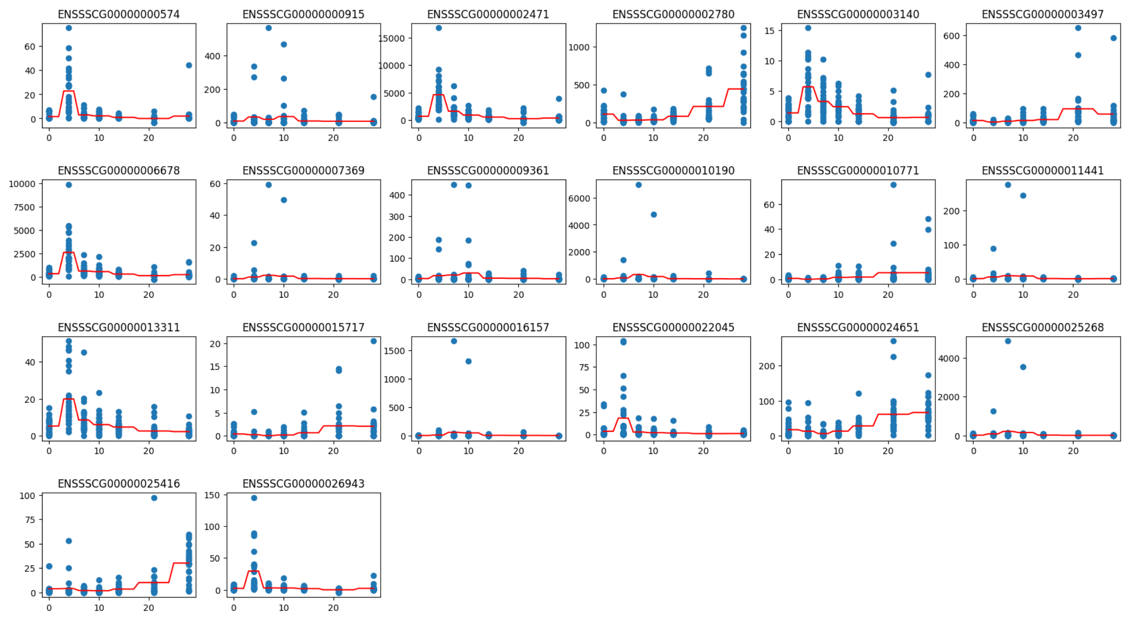
[16]:
```
def regress(df, gene, n):
    # individual models
    model1 = LinearRegression()

    x = df['day'].values.reshape(-1,1)
    y = df[gene].values.reshape(-1,1).ravel()
    model1.fit(x,y)

    lin = np.arange(0,29).reshape(-1, 1)
    preds = model1.predict(lin)

    ax = plt.subplot(5, 6, n + 1)
    plt.scatter(df['day'], df[gene])
    plt.plot(lin, preds, color='red')
    plt.title(gene)


plt.figure(figsize=(22, 15))
plt.subplots_adjust(hspace=0.5)

for i, gene in enumerate(gdn_keep.columns):
    if gene != 'dpi':

        regress(poly_df2, gene, i)
```



[17]:
```
df_mods = []

def regress(df, gene, n):

    param_grid = {

        'max_depth': [5, 10, 20, None],
        'min_samples_split': [2, 5, 10],
        'min_samples_leaf': [1, 2, 4],
        'max_features': ['sqrt', 'log2', None]
    }

    # Create the Decision Tree Regressor object
    dt = DecisionTreeRegressor()

    # Create a K-Fold cross-validator with 5 splits
    kf = KFold(n_splits=2, shuffle=True, random_state=42)

    # Create the Grid Search object with the parameter grid and K-Fold␣
 ↪cross-validator
    grid_search = GridSearchCV(dt, param_grid, cv=kf, n_jobs=3)
    x = df['day'].values.reshape(-1,1)
    y = df[gene].values.reshape(-1,1).ravel()

    # Fit the Grid Search object to the data
    grid_search.fit(x, y)

    # Print the best parameters and score
    best_params = grid_search.best_params_

    df_func = DecisionTreeRegressor(max_depth = best_params['max_depth'],
                                    min_samples_split =␣
 ↪best_params['min_samples_split'],
                                    min_samples_leaf =␣
 ↪best_params['min_samples_leaf'],
                                    max_features = best_params['max_features'])

    df_mods.append(df_func)

    df_func.fit(x,y)

    lin = np.arange(0,29).reshape(-1, 1)
    preds = df_func.predict(lin)

    ax = plt.subplot(5, 6, n + 1)
    plt.scatter(df['day'], df[gene])
    plt.plot(lin, preds, color='red')
    plt.title(gene)


plt.figure(figsize=(22, 15))
plt.subplots_adjust(hspace=0.5)

for i, gene in enumerate(gdn_keep.columns):

    if gene != 'dpi':

        regress(poly_df2, gene, i)
```



[18]:
```python
rf_mods = []

def regress(df, gene, n):
    # Define the parameter grid to search over
    param_grid = {
        'n_estimators': [100, 200, 500],
        'max_features': ['sqrt', 'log2', None],
        'max_depth': [10, 20, 30, None]
    }

    # Create the Random Forest regressor object
    rf = RandomForestRegressor()

    # Create a K-Fold cross-validator with 5 splits
    kf = KFold(n_splits=2, shuffle=True, random_state=42)

    # Create the Grid Search object with the parameter grid and K-Fold␣
 ↪cross-validator
    grid_search = GridSearchCV(rf, param_grid, cv=kf, n_jobs=3)

    x = df['day'].values.reshape(-1,1)
    y = df[gene].values.reshape(-1,1).ravel()

    # Fit the Grid Search object to the data
    grid_search.fit(x, y)

    best_params = grid_search.best_params_
    # create a new KNN regressor with the best hyperparameters
    rf_func = RandomForestRegressor(n_estimators=best_params['n_estimators'],
                                   max_features=best_params['max_features'],
                                     max_depth=best_params['max_depth'],
                                     n_jobs=3)

    rf_mods.append(rf_func)

    rf_func.fit(x,y)

    lin = np.arange(0,29).reshape(-1, 1)
    preds = rf_func.predict(lin)

    ax = plt.subplot(5, 6, n + 1)
    plt.scatter(df['day'], df[gene])
    plt.plot(lin, preds, color='red')
    plt.title(gene)


plt.figure(figsize=(22, 15))
plt.subplots_adjust(hspace=0.5)

for i, gene in enumerate(gdn_keep.columns):

    if gene != 'dpi':

        regress(poly_df2, gene, i)
```



[19]:
```
# from sklearn.model_selection import train_test_split

# train, test = train_test_split(poly_df2, test_size=0.2)

# X_train = train.drop('day', axis=1)
# y_train = train['day']
# X_test = train.drop('day', axis=1)
# y_test = train['day']
```

[20]:
```
# ## Doing a proportional split
# # for example if i have 100 samples and do an 80/20 split
# # of those 80 on the train

# # percentage of data for training
# train_pct = 0.8

# groups = poly_df2.groupby('gene')

# # randomly sample the data within each group
# def sample_group(group):
#     n_samples = len(group)
#     n_train = int(n_samples * train_pct)
#     train_idx = np.random.choice(group.index, size=n_train, replace=False)
#     test_idx = group.index.difference(train_idx)
#     return {'train': group.loc[train_idx], 'test': group.loc[test_idx]}

# # apply sample_group to each group and combine the results into a dictionary
# group_samples = groups.apply(sample_group).to_dict()

# # combine into single df
# train_data = pd.concat([group_samples[group]['train'] for group in␣
 ↪group_samples]).drop('gene', axis=1)
# test_data = pd.concat([group_samples[group]['test'] for group in␣
 ↪group_samples]).drop('gene', axis=1)
```

[21]:
```
# X_train = train_data.drop('ge', axis=1)
# y_train = train_data['ge']
# X_test = test_data.drop('ge', axis=1)
# y_test = test_data['ge']
```

[22]:
```
# from sklearn.ensemble import VotingRegressor
# from sklearn.linear_model import LinearRegression
# from sklearn.tree import DecisionTreeRegressor
# from sklearn.ensemble import RandomForestRegressor
# # individual models
# model1 = LinearRegression()
# model2 = DecisionTreeRegressor()
# model3 = RandomForestRegressor()

# ensemble_model = VotingRegressor(estimators=[('lr', model1),
#                                              ('dt', model2),
#                                              ('rf', model3)])

# ensemble_model.fit(X_train, y_train)

# # Evaluate test data
# ensemble_model.score(X_test, y_test)
```

[ ]:

```
```