scikit-learn Cross-validation

Lecture 15

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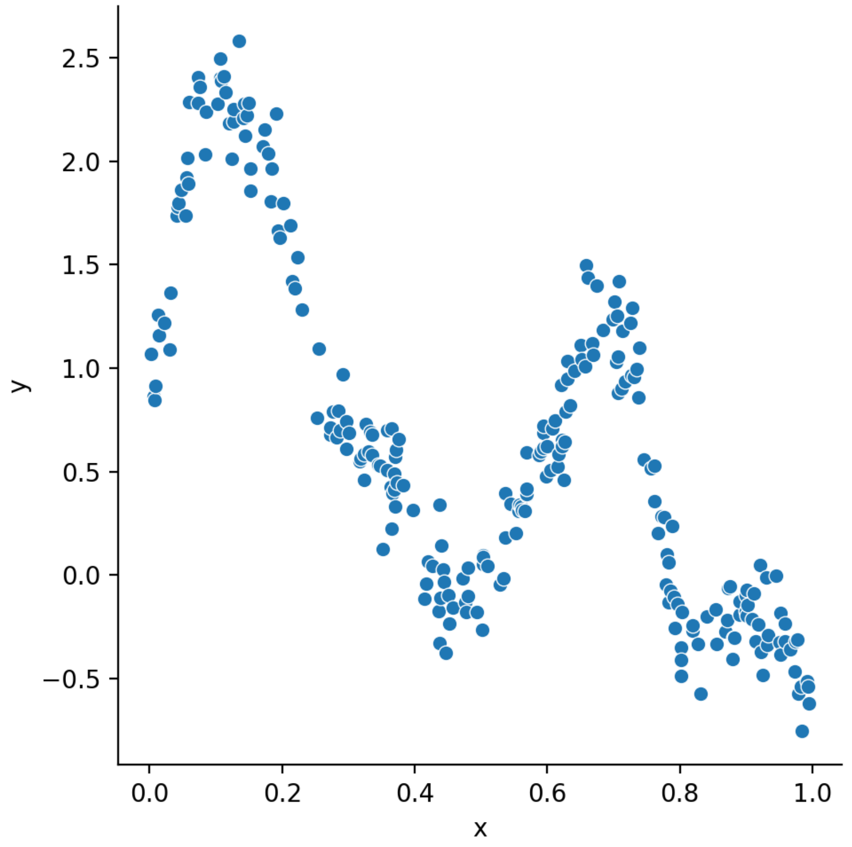
Pipelines

From last time

We will now look at another flavor of regression model, that involves preprocessing and a hyperparameter - namely polynomial regression.

```python
df = pd.read_csv("data/gp.csv")
sns.relplot(data=df, x="x", y="y")
```



Pipelines

You may have noticed that `PolynomialFeatures` takes a model matrix as input and returns a new model matrix as output which is then used as the input for `LinearRegression`. This is not an accident, and by structuring the library in this way sklearn is designed to enable the connection of these steps together, into what sklearn calls a *pipeline*.

```python
from sklearn.pipeline import make_pipeline

p = make_pipeline(
  PolynomialFeatures(degree=4),
  LinearRegression()
)
p
```

```
Pipeline(steps=[('polynomialfeatures', PolynomialFeatures(degree=4)),
                ('linearregression', LinearRegression())])
```

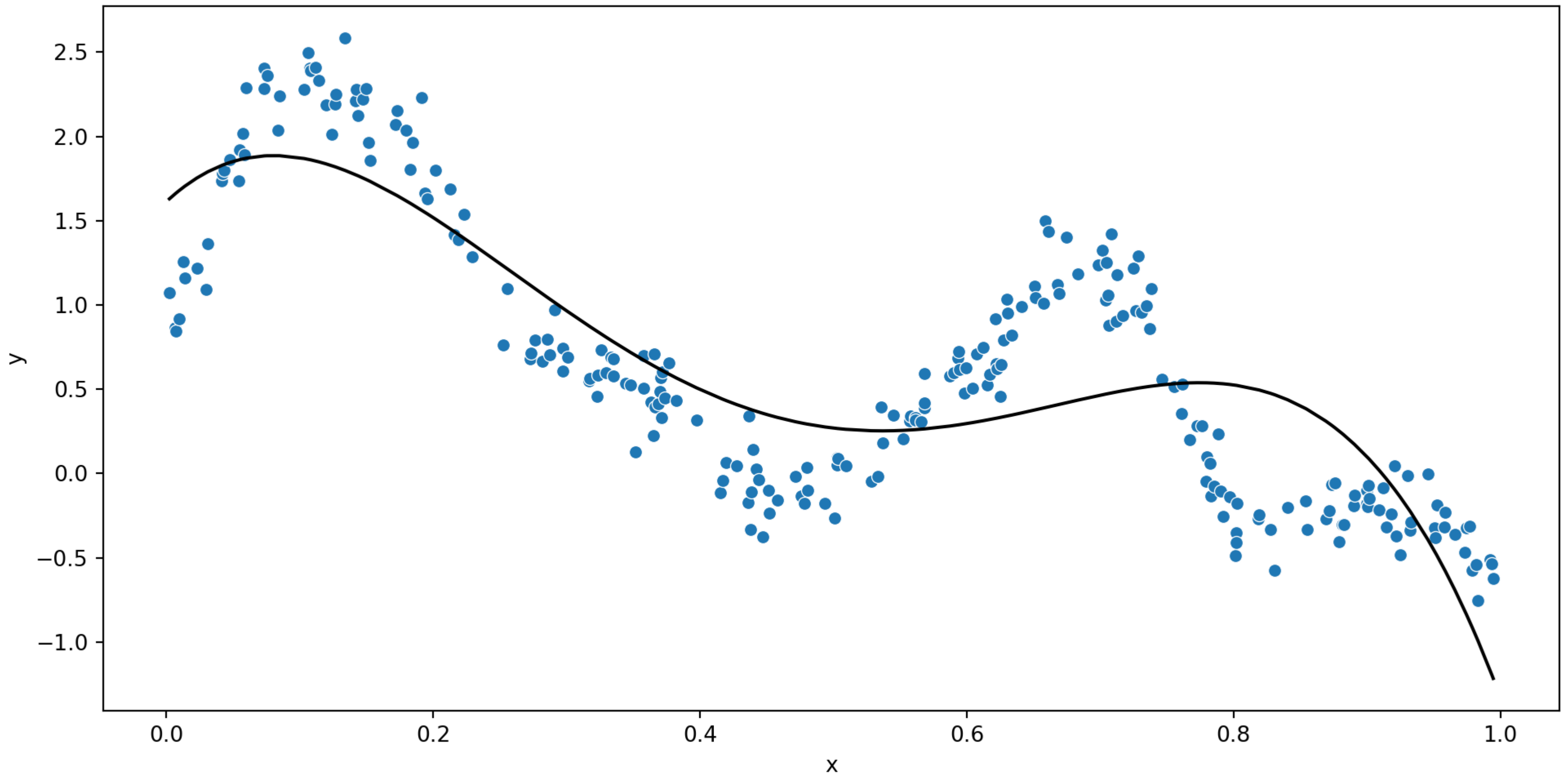
Using Pipelines

Once constructed, this object can be used just like our previous `LinearRegression` model (i.e. fit to our data and then used for prediction)

```python
p = p.fit(X = df[["x"]], y = df.y)
p.predict(X = df[["x"]])
```

```
array([ 1.62957,  1.65735,  1.66105,  1.6778 ,  1.69667,  1.70475,  1.7528 ,  1.78471,  1.7905 ,  1.8269 ,
        1.8844 ,  1.88527,  1.88577,  1.88544,  1.86891,  1.86365,  1.86253,  1.86047,  1.85378,  1.84938,
        1.7439 ,  1.73804,  1.73357,  1.65528,  1.64812,  1.61868,  1.60413,  1.59604,  1.56081,  1.55036,
        1.11776,  1.11522,  1.09595,  1.0645 ,  1.04672,  1.03663,  1.01407,  0.98209,  0.98082,  0.96177,
        0.73538,  0.71815,  0.70047,  0.67234,  0.67229,  0.64783,  0.64051,  0.63727,  0.63526,  0.62323,
        0.44178,  0.43291,  0.40958,  0.3848 ,  0.38289,  0.38068,  0.37915,  0.3761 ,  0.36933,  0.36493,
        0.27632,  0.26899,  0.26761,  0.26726,  0.26716,  0.26242,  0.25405,  0.25335,  0.25323,  0.25323,
        0.26486,  0.26489,  0.28177,  0.28525,  0.28861,  0.28918,  0.29004,  0.29445,  0.2956 ,  0.30233,
        0.33711,  0.34111,  0.34141,  0.34707,  0.35926,  0.37678,  0.37775,  0.38885,  0.39078,  0.39518,
        0.4751 ,  0.47762,  0.48382,  0.48474,  0.49067,  0.50203,  0.50448,  0.50675,  0.5096 ,  0.51457,
        0.53839,  0.53823,  0.53757,  0.53749,  0.5365 ,  0.53481,  0.53372,  0.53274,  0.52872,  0.52378,
        0.38104,  0.31132,  0.29845,  0.28774,  0.27189,  0.2524 ,  0.23846,  0.22915,  0.17792,  0.17355,
       -0.09117, -0.10696, -0.13889, -0.20218, -0.22105, -0.23335, -0.39046, -0.46281, -0.47156, -0.48247, -
       -1.16341, -1.19337, -1.21549])
```

```python
plt.figure(layout="constrained")
sns.scatterplot(data=df, x="x", y="y")
sns.lineplot(x=df.x, y=p.predict(X = df[["x"]]), color="k")
plt.show()
```



Model coefficients (or other attributes)

The attributes of pipeline steps are not directly accessible, but can be accessed via the `steps` or `named_steps` attributes,

```
p.coef_
```

```
Error: AttributeError: 'Pipeline' object has no attribute 'coef_'
```

```
p.steps
```

```
[('polynomialfeatures', PolynomialFeatures(degree=4)), ('linearregression', LinearRegression())]
```

```
p.steps[1][1].coef_
```

```
array([  0.       ,   7.39051, -57.67175, 102.72227, -55.38181])
```

```
p.named_steps["linearregression"].intercept_
```

```
1.6136636604768615
```

Other useful bits

```python
p.steps[0][1].get_feature_names_out()
```

```
array(['1', 'x', 'x^2', 'x^3', 'x^4'], dtype=object)
```

```python
p.steps[1][1].get_params()
```

```
{'copy_X': True, 'fit_intercept': True, 'n_jobs': None, 'positive': False}
```

Anyone notice a problem?

```python
p.steps[1][1].rank_
```

```
4
```

```python
p.steps[1][1].n_features_in_
```

```
5
```

What about step parameters?

By accessing each step we can adjust their parameters (via `set_params()`),

```python
p.named_steps["linearregression"].get_params()
```

```
{'copy_X': True, 'fit_intercept': True, 'n_jobs': None, 'positive': False}
```

```python
p.named_steps["linearregression"].set_params(
  fit_intercept=False
)
```

```
LinearRegression(fit_intercept=False)
```

```python
p.fit(X = df[["x"]], y = df.y)
```

```
Pipeline(steps=[('polynomialfeatures', PolynomialFeatures(degree=4)),
                ('linearregression', LinearRegression(fit_intercept=False))])
```

```python
p.named_steps["linearregression"].intercept_
```

```
0.0
```

```python
p.named_steps["linearregression"].coef_
```

```
array([  1.61366,   7.39051, -57.67175, 102.72227, -55.38181])
```

Pipeline parameter names

These parameters can also be directly accessed at the pipeline level, names are constructed as step name + __ + parameter name:

```
p.get_params()
```

```
{'memory': None, 'steps': [('polynomialfeatures', PolynomialFeatures(degree=4)), ('linearregression', Linear
```

```
p.set_params(
  linearregression__fit_intercept=True,
  polynomialfeatures__include_bias=False
)
```

```
Pipeline(steps=[('polynomialfeatures',
                 PolynomialFeatures(degree=4, include_bias=False)),
                ('linearregression', LinearRegression())])
```

```python
p.fit(X = df[["x"]], y = df.y)
```

```
Pipeline(steps=[('polynomialfeatures',
                 PolynomialFeatures(degree=4, include_bias=False)),
                ('linearregression', LinearRegression())])
```

```python
p.named_steps["polynomialfeatures"].get_feature_names_out()
```

```
array(['x', 'x^2', 'x^3', 'x^4'], dtype=object)
```

```python
p.named_steps["linearregression"].intercept_
```

```
1.6136636604768375
```

```python
p.named_steps["linearregression"].coef_
```

```
array([  7.39051, -57.67175, 102.72227, -55.38181])
```

Column Transformers

Column Transformers

Are a tool for selectively applying transformer(s) to column(s) of an array or DataFrame, they function in a way that is similar to a pipeline and similarly have a make helper function.

```python
from sklearn.compose import make_column_transformer
from sklearn.preprocessing import StandardScaler, OneHotEncoder
```

```python
ct = make_column_transformer(
  (StandardScaler(), ["volume"]),
  (OneHotEncoder(), ["cover"]),
).fit(
  books
)
```

```python
ct.get_feature_names_out()
```

```
array(['standardscaler__volume', 'onehotencoder__cove
```

```python
ct.transform(books)
```

```
array([[ 0.12101,  1.      ,  0.      ],
       [ 0.51997,  1.      ,  0.      ],
       [ 0.85192,  1.      ,  0.      ],
       [-1.84637,  1.      ,  0.      ],
       [-0.43936,  1.      ,  0.      ],
       [-0.62209,  1.      ,  0.      ],
       [ 1.16561,  1.      ,  0.      ],
       [-1.31951,  0.      ,  1.      ],
       [ 0.3281 ,  0.      ,  1.      ],
       [ 0.25501,  0.      ,  1.      ],
       [ 1.96962,  0.      ,  1.      ],
       [-1.29819,  0.      ,  1.      ],
       [ 0.50169,  0.      ,  1.      ],
       [-0.76218,  0.      ,  1.      ],
       [ 0.57478,  0.      ,  1.      ]])
```

Keeping or dropping other columns

One addition important argument is `remainder` which determines what happens to unspecified columns. The default is `"drop"` which is why `weight` was removed, the alternative is `"passthrough"` which retains untransformed columns.

```python
ct = make_column_transformer(
  (StandardScaler(), ["volume"]),
  (OneHotEncoder(), ["cover"]),
  remainder = "passthrough"
).fit(
  books
)
```

```python
ct.get_feature_names_out()
```

```
array(['standardscaler__volume', 'onehotencoder__cove
```

```python
ct.transform(books)
```

```
array([[   0.12101,    1.     ,    0.     ,  800.
       [   0.51997,    1.     ,    0.     ,  950.
       [   0.85192,    1.     ,    0.     , 1050.
       [  -1.84637,    1.     ,    0.     ,  350.
       [  -0.43936,    1.     ,    0.     ,  750.
       [  -0.62209,    1.     ,    0.     ,  600.
       [   1.16561,    1.     ,    0.     , 1075.
       [  -1.31951,    0.     ,    1.     ,  250.
       [   0.3281 ,    0.     ,    1.     ,  700.
       [   0.25501,    0.     ,    1.     ,  650.
       [   1.96962,    0.     ,    1.     ,  975.
       [  -1.29819,    0.     ,    1.     ,  350.
       [   0.50169,    0.     ,    1.     ,  950.
       [  -0.76218,    0.     ,    1.     ,  425.
       [   0.57478,    0.     ,    1.     ,  725.
```

Column selection

One lingering issue with the above approach is that we've had to hard code the column names (or use indexes). Often we want to select columns based on their dtype (e.g. categorical vs numerical) this can be done via pandas or sklearn,

```python
from sklearn.compose import make_column_selector
```

```python
ct = make_column_transformer(
  ( StandardScaler(),
    make_column_selector(
      dtype_include=np.number
    )
  ),
  ( OneHotEncoder(),
    make_column_selector(
      dtype_include=[object, bool]
    )
  )
)
```

```python
ct = make_column_transformer(
  ( StandardScaler(),
    books.select_dtypes(
      include=['number']
    ).columns
  ),
  ( OneHotEncoder(),
    books.select_dtypes(
      include=['object']
    ).columns
  )
)
```

`make_column_selector()` also supports selecting via `pattern` or excluding via `dtype_exclude`

```python
ct.fit_transform(books)
```

```
array([[ 0.12101,  0.35936,  1.     ,  0.     ],
       [ 0.51997,  0.9369 ,  1.     ,  0.     ],
       [ 0.85192,  1.32193,  1.     ,  0.     ],
       [-1.84637, -1.37326,  1.     ,  0.     ],
       [-0.43936,  0.16685,  1.     ,  0.     ],
       [-0.62209, -0.4107 ,  1.     ,  0.     ],
       [ 1.16561,  1.41818,  1.     ,  0.     ],
       [-1.31951, -1.75829,  0.     ,  1.     ],
       [ 0.3281 , -0.02567,  0.     ,  1.     ],
       [ 0.25501, -0.21818,  0.     ,  1.     ],
       [ 1.96962,  1.03316,  0.     ,  1.     ],
       [-1.29819, -1.37326,  0.     ,  1.     ],
       [ 0.50169,  0.9369 ,  0.     ,  1.     ],
       [-0.76218, -1.08449,  0.     ,  1.     ],
       [ 0.57478,  0.07059,  0.     ,  1.     ]])
```

```python
ct.get_feature_names_out()
```

```
array(['standardscaler__volume', 'standardscaler__we
```

```python
ct.fit_transform(books)
```

```
array([[ 0.12101,  0.35936,  1.     ,  0.     ],
       [ 0.51997,  0.9369 ,  1.     ,  0.     ],
       [ 0.85192,  1.32193,  1.     ,  0.     ],
       [-1.84637, -1.37326,  1.     ,  0.     ],
       [-0.43936,  0.16685,  1.     ,  0.     ],
       [-0.62209, -0.4107 ,  1.     ,  0.     ],
       [ 1.16561,  1.41818,  1.     ,  0.     ],
       [-1.31951, -1.75829,  0.     ,  1.     ],
       [ 0.3281 , -0.02567,  0.     ,  1.     ],
       [ 0.25501, -0.21818,  0.     ,  1.     ],
       [ 1.96962,  1.03316,  0.     ,  1.     ],
       [-1.29819, -1.37326,  0.     ,  1.     ],
       [ 0.50169,  0.9369 ,  0.     ,  1.     ],
       [-0.76218, -1.08449,  0.     ,  1.     ],
       [ 0.57478,  0.07059,  0.     ,  1.     ]])
```

```python
ct.get_feature_names_out()
```

```
array(['standardscaler__volume', 'standardscaler__we
```

Demo 1 - Putting it together Interaction model

Cross validation & hyper parameter tuning

Ridge regression

One way to expand on the idea of least squares regression is to modify the loss function. One such approach is known as Ridge regression, which adds a scaled penalty for the sum of the squares of the βs to the least squares loss.

$$\underset{\boldsymbol{\beta}}{\operatorname{argmin}} \; \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta}\|^2 + \lambda(\boldsymbol{\beta}^T\boldsymbol{\beta})$$

```
d = pd.read_csv("data/ridge.csv")
d
```

```
            y        x1        x2        x3        x4 x5
0   -0.151710  0.353658  1.633932  0.553257  1.415731  A
1    3.579895  1.311354  1.457500  0.072879  0.330330  B
2    0.768329 -0.744034  0.710362 -0.246941  0.008825  B
3    7.788646  0.806624 -0.228695  0.408348 -2.481624  B
4    1.394327  0.837430 -1.091535 -0.860979 -0.810492  A
..        ...       ...       ...       ...       ... ..
495 -0.204932 -0.385814 -0.130371 -0.046242  0.004914  A
496  0.541988  0.845885  0.045291  0.171596  0.332869  A
497 -1.402627 -1.071672 -1.716487 -0.319496 -1.163740  C
498 -0.043645  1.744800 -0.010161  0.422594  0.772606  A
499 -1.550276  0.910775 -1.675396  1.921238 -0.232189  B

[500 rows x 6 columns]
```

dummy coding

```
d = pd.get_dummies(d)
d
```

```
            y        x1        x2        x3        x4  x5_A  x5_B  x5_C  x5_D
0   -0.151710  0.353658  1.633932  0.553257  1.415731     1     0     0     0
1    3.579895  1.311354  1.457500  0.072879  0.330330     0     1     0     0
2    0.768329 -0.744034  0.710362 -0.246941  0.008825     0     1     0     0
3    7.788646  0.806624 -0.228695  0.408348 -2.481624     0     1     0     0
4    1.394327  0.837430 -1.091535 -0.860979 -0.810492     1     0     0     0
..        ...       ...       ...       ...       ...   ...   ...   ...   ...
495 -0.204932 -0.385814 -0.130371 -0.046242  0.004914     1     0     0     0
496  0.541988  0.845885  0.045291  0.171596  0.332869     1     0     0     0
497 -1.402627 -1.071672 -1.716487 -0.319496 -1.163740     0     0     1     0
498 -0.043645  1.744800 -0.010161  0.422594  0.772606     1     0     0     0
499 -1.550276  0.910775 -1.675396  1.921238 -0.232189     0     1     0     0

[500 rows x 9 columns]
```

Fitting a ridge regession model

The `linear_model` submodule also contains the `Ridge` model which can be used to fit a ridge regression. Usage is identical other than `Ridge()` takes the parameter `alpha` to specify the regularization parameter.

```python
from sklearn.linear_model import Ridge, LinearRegression

X, y = d.drop(["y"], axis=1), d.y

rg = Ridge(fit_intercept=False, alpha=10).fit(X, y)
lm = LinearRegression(fit_intercept=False).fit(X, y)
```

```python
rg.coef_
```

```
array([ 0.97809,  1.96215,  0.00172, -2.94457,  0.45
```

```python
mean_squared_error(y, rg.predict(X))
```

```
0.019101431349883385
```

```python
lm.coef_
```

```
array([ 0.99505,  2.00762,  0.00232, -3.00088,  0.49
```

```python
mean_squared_error(y, lm.predict(X))
```

```
0.009872435924102045
```

Generally for a Ridge (or Lasso) model it is important to scale the features before fitting (i.e. `StandardScaler()`) -

Test-Train split

The most basic form of CV is to split the data into a testing and training set, this can be achieved using `train_test_split` from the `model_selection` submodule.

```python
from sklearn.model_selection import train_test_split

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.2, random_state=1234)
```

```python
X.shape
```

```
(500, 8)
```

```python
y.shape
```

```
(500,)
```

```python
X_train.shape
```

```
(400, 8)
```

```python
y_train.shape
```

```
(400,)
```

```python
X_test.shape
```

```
(100, 8)
```

```python
y_test.shape
```

```
(100,)
```

```
X_train
```

```
           x1        x2        x3        x4  x5_A  x!
296 -0.261142 -0.887193 -0.441300  0.053902     0
220  0.155596  0.551363  0.749117  0.875181     0
0    0.353658  1.633932  0.553257  1.415731     1
255 -1.206309 -0.073534 -1.920777 -0.554861     1
335 -0.380790 -0.117404 -0.037709  0.202757     0
..        ...       ...       ...       ...   ...
204 -2.646094  1.170804 -0.185098  0.165830     0
53  -0.483511  0.452531  0.223226 -0.753872     0
294 -1.424818 -0.396870 -0.595927 -1.114747     1
211 -1.000845 -0.842665  0.407765  0.375650     0
303  1.037404 -0.961266  0.433180  0.890055     0

[400 rows x 8 columns]
```

```
y_train
```

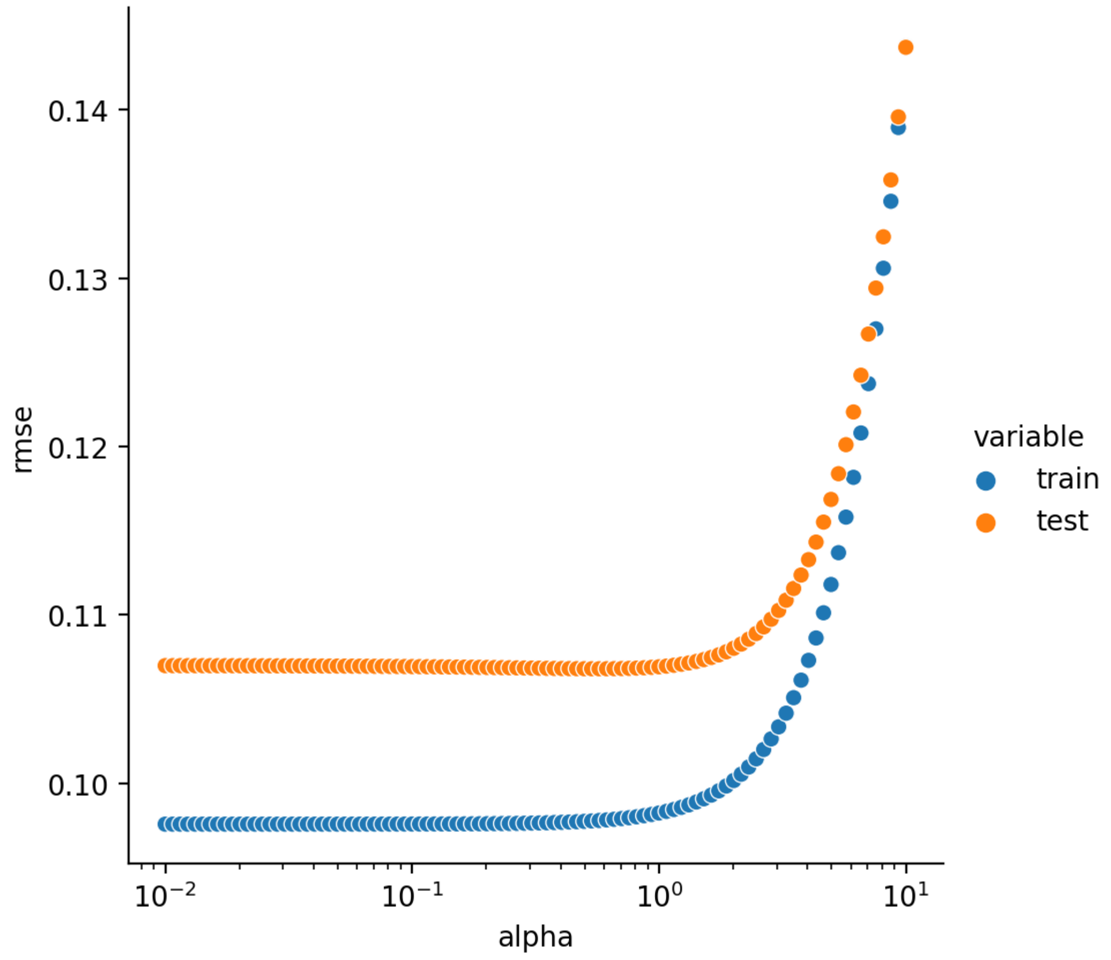
```
296   -2.462944
220   -1.760134
0     -0.151710
255    0.668016
335   -1.178652
         ...
204   -0.657622
53     2.831201
294    1.566109
211   -3.711740
303   -3.552971
Name: y, Length: 400, dtype: float64
```

Train vs Test rmse

```
alpha = np.logspace(-2,1, 100)
train_rmse = []
test_rmse = []

for a in alpha:
    rg = Ridge(alpha=a).fit(X_train, y_train)

    train_rmse.append(
      mean_squared_error(
        y_train, rg.predict(X_train), squared=Fa
      )
    )
    test_rmse.append(
      mean_squared_error(
        y_test, rg.predict(X_test), squared=Fals
      )
    )

res = pd.DataFrame(
  data = {"alpha": alpha,
          "train": train_rmse,
          "test": test_rmse}
)
```

```
        alpha     train      test
0    0.010000  0.097568  0.106985
1    0.010723  0.097568  0.106984
2    0.011498  0.097568  0.106984
3    0.012328  0.097568  0.106983
4    0.013219  0.097568  0.106983
..        ...       ...       ...
95   7.564633  0.126990  0.129414
96   8.111308  0.130591  0.132458
97   8.697490  0.134568  0.135838
98   9.326033  0.138950  0.139581
99  10.000000  0.143764  0.143715

[100 rows x 3 columns]
```

```python
sns.relplot(
  x="alpha", y="rmse", hue="variable", data = pd.melt(res, id_vars=["alpha"],value_name="rmse")
).set(
  xscale="log"
)
```



Best alpha?

```python
min_i = np.argmin(res.train)
min_i
```

```
0
```

```python
res.iloc[[min_i],:]
```

```
   alpha     train      test
0   0.01  0.097568  0.106985
```

```python
min_i = np.argmin(res.test)
min_i
```

```
58
```

```python
res.iloc[[min_i],:]
```

```
       alpha     train    test
58  0.572237  0.097787  0.1068
```

k-fold cross validation

The previous approach was relatively straight forward, but it required a fair bit of book keeping to implement and we only examined a single test/train split. If we would like to perform k-fold cross validation we can use `cross_val_score` from the `model_selection` submodule.

```python
from sklearn.model_selection import cross_val_score

cross_val_score(
  Ridge(alpha=0.59, fit_intercept=False),
  X, y,
  cv=5,
  scoring="neg_root_mean_squared_error"
)
```

```
array([-0.09364, -0.09995, -0.10474, -0.10273, -0.10597])
```

🚩🚩🚩 Note that the default k-fold cross validation used here does not shuffle your data which can be massively

Controling k-fold behavior

Rather than providing `cv` as an integer, it is better to specify a cross-validation scheme directly (with additional options). Here we will use the `KFold` class from the `model_selection` submodule.

```python
from sklearn.model_selection import KFold

cross_val_score(
  Ridge(alpha=0.59, fit_intercept=False),
  X, y,
  cv = KFold(n_splits=5, shuffle=True, random_state=1234),
  scoring="neg_root_mean_squared_error"
)
```

```
array([-0.10658, -0.104  , -0.1037 , -0.10125, -0.09228])
```

KFold object

`KFold()` returns a class object which provides the method `split()` which in turn is a generator that returns a tuple with the indexes of the training and testing selects for each fold given a model matrix `X`,

```python
ex = pd.DataFrame(data = list(range(10)), columns=["x"])
```

```python
cv = KFold(5)
for train, test in cv.split(ex):
  print(f'Train: {train} | test: {test}')
```

```
Train: [2 3 4 5 6 7 8 9] | test: [0 1]
Train: [0 1 4 5 6 7 8 9] | test: [2 3]
Train: [0 1 2 3 6 7 8 9] | test: [4 5]
Train: [0 1 2 3 4 5 8 9] | test: [6 7]
Train: [0 1 2 3 4 5 6 7] | test: [8 9]
```

```python
cv = KFold(5, shuffle=True, random_state=1234)
for train, test in cv.split(ex):
  print(f'Train: {train} | test: {test}')
```

```
Train: [0 1 3 4 5 6 8 9] | test: [2 7]
Train: [0 2 3 4 5 6 7 8] | test: [1 9]
Train: [1 2 3 4 5 6 7 9] | test: [0 8]
Train: [0 1 2 3 6 7 8 9] | test: [4 5]
Train: [0 1 2 4 5 7 8 9] | test: [3 6]
```

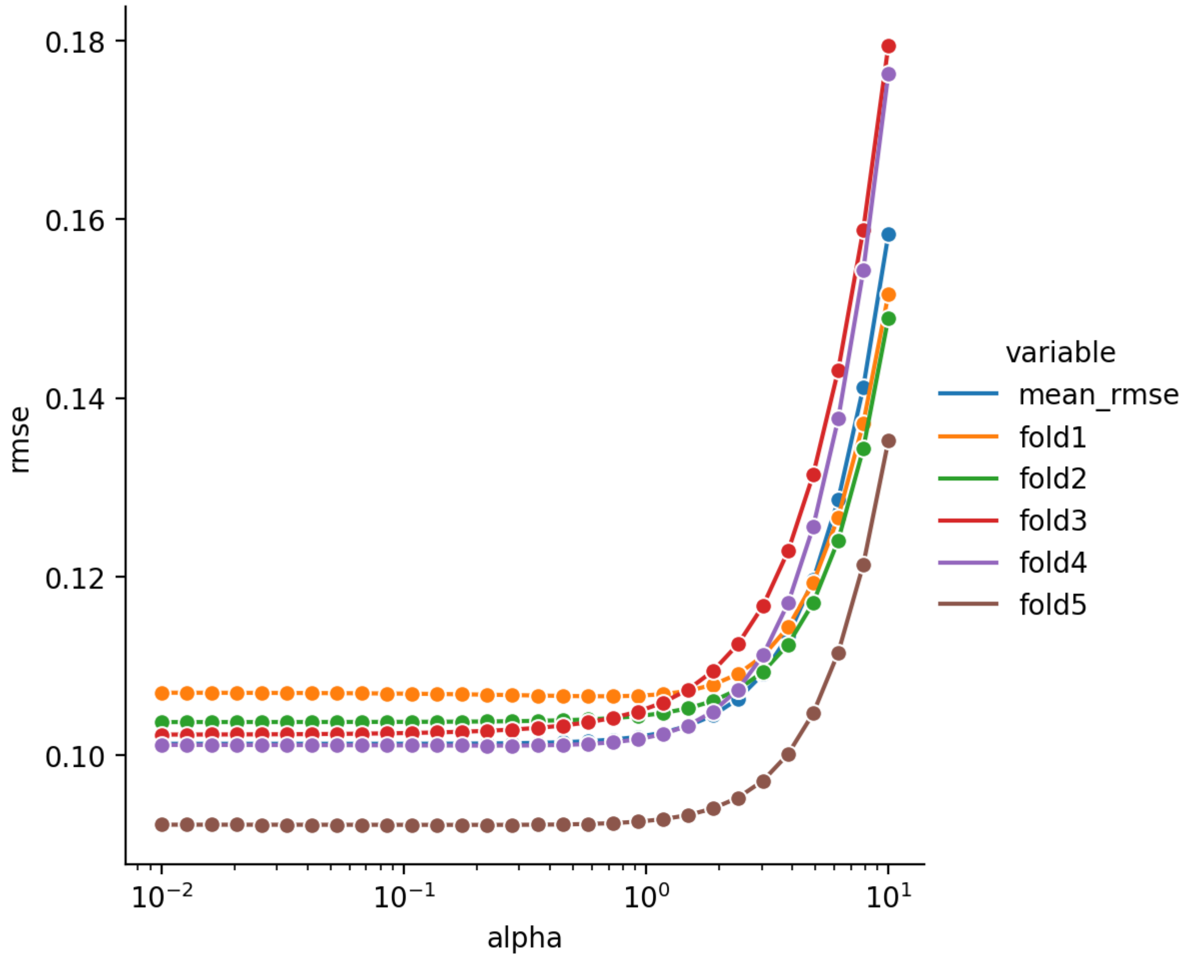
Train vs Test rmse (again)

```python
alpha = np.logspace(-2,1, 30)
test_mean_rmse = []
test_rmse = []
cv = KFold(n_splits=5, shuffle=True, random_state=1234)

for a in alpha:
    rg = Ridge(fit_intercept=False, alpha=a).fit(X_train, y_train)

    scores = -1 * cross_val_score(
      rg, X, y,
      cv = cv,
      scoring="neg_root_mean_squared_error"
    )
    test_mean_rmse.append(np.mean(scores))
    test_rmse.append(scores)

res = pd.DataFrame(
    data = np.c_[alpha, test_mean_rmse, test_rmse],
    columns = ["alpha", "mean_rmse"] + ["fold" + str(i) for i in range(1,6) ]
)
```

```
res
```

```
       alpha  mean_rmse     fold1     fold2     fold3     fold4     fold5
0   0.010000   0.101257  0.106979  0.103691  0.102288  0.101130  0.092195
1   0.012690   0.101257  0.106976  0.103692  0.102292  0.101129  0.092194
2   0.016103   0.101256  0.106971  0.103692  0.102298  0.101126  0.092194
3   0.020434   0.101256  0.106966  0.103693  0.102306  0.101123  0.092193
4   0.025929   0.101256  0.106959  0.103694  0.102316  0.101120  0.092191
5   0.032903   0.101256  0.106951  0.103696  0.102328  0.101116  0.092190
6   0.041753   0.101256  0.106940  0.103698  0.102344  0.101110  0.092188
7   0.052983   0.101256  0.106927  0.103701  0.102365  0.101104  0.092186
8   0.067234   0.101257  0.106911  0.103704  0.102391  0.101096  0.092184
9   0.085317   0.101259  0.106890  0.103709  0.102426  0.101088  0.092181
10  0.108264   0.101262  0.106865  0.103716  0.102471  0.101078  0.092178
11  0.137382   0.101267  0.106835  0.103725  0.102529  0.101069  0.092176
12  0.174333   0.101276  0.106800  0.103739  0.102607  0.101060  0.092174
13  0.221222   0.101291  0.106758  0.103758  0.102710  0.101055  0.092175
14  0.280722   0.101317  0.106712  0.103786  0.102848  0.101059  0.092180
15  0.356225   0.101360  0.106663  0.103828  0.103036  0.101078  0.092193
16  0.452035   0.101430  0.106617  0.103890  0.103293  0.101128  0.092221
17  0.573615   0.101544  0.106584  0.103984  0.103650  0.101229  0.092273
18  0.727895   0.101729  0.106580  0.104128  0.104149  0.101420  0.092367
19  0.923671   0.102026  0.106639  0.104348  0.104856  0.101757  0.092530
20  1.172102   0.102501  0.106809  0.104690  0.105864  0.102334  0.092805
21  1.487352   0.103253  0.107174  0.105220  0.107314  0.103295  0.093263
```

```python
sns.relplot(
  x="alpha", y="rmse", hue="variable", data=res.melt(id_vars=["alpha"], value_name="rmse"),
  marker="o", kind="line"
).set(
  xscale="log"
)
```



Best alpha? (again)

```
i = res.drop(
  ["alpha"], axis=1
).agg(
  np.argmin
).to_numpy()

i = np.sort(np.unique(i))

res.iloc[ i, : ]
```

```
       alpha  mean_rmse     fold1     fold2     fold3     fold4     fold5
0   0.010000   0.101257  0.106979  0.103691  0.102288  0.101130  0.092195
5   0.032903   0.101256  0.106951  0.103696  0.102328  0.101116  0.092190
12  0.174333   0.101276  0.106800  0.103739  0.102607  0.101060  0.092174
13  0.221222   0.101291  0.106758  0.103758  0.102710  0.101055  0.092175
18  0.727895   0.101729  0.106580  0.104128  0.104149  0.101420  0.092367
```

Aside - Available metrics

For most of the cross validation functions we pass in a string instead of a scoring function from the metrics submodule - if you are interested in seeing the names of the possible metrics, these are available via the `sklearn.metrics.SCORERS` dictionary,

```
np.array( sorted(
  sklearn.metrics.SCORERS.keys()
) )
```

```
array(['accuracy', 'adjusted_mutual_info_score', 'adjusted_rand_score', 'average_precision', 'balanced_accur
       'f1_samples', 'f1_weighted', 'fowlkes_mallows_score', 'homogeneity_score', 'jaccard', 'jaccard_macro'
       'mutual_info_score', 'neg_brier_score', 'neg_log_loss', 'neg_mean_absolute_error', 'neg_mean_absolute
       'neg_mean_squared_error', 'neg_mean_squared_log_error', 'neg_median_absolute_error', 'neg_negative_li
       'positive_likelihood_ratio', 'precision', 'precision_macro', 'precision_micro', 'precision_samples',
       'recall_samples', 'recall_weighted', 'roc_auc', 'roc_auc_ovo', 'roc_auc_ovo_weighted', 'roc_auc_ovr',
```

Grid Search

We can further reduce the amount of code needed if there is a specific set of parameter values we would like to explore using cross validation. This is done using the `GridSearchCV` function from the `model_selection` submodule.

```python
from sklearn.model_selection import GridSearchCV

gs = GridSearchCV(
  Ridge(fit_intercept=False),
  {"alpha": np.logspace(-2, 1, 30)},
  cv = KFold(5, shuffle=True, random_state=1234),
  scoring = "neg_root_mean_squared_error"
).fit(
  X, y
)
```

```python
gs.best_index_
```

```
5
```

```python
gs.best_params_
```

```
{'alpha': 0.03290344562312668}
```

```python
gs.best_score_
```

```
-0.10125611767453653
```

`best_estimator_` attribute

If `refit = True` (the default) with `GridSearchCV()` then the `best_estimator_` attribute will be available which gives direct access to the "best" model or pipeline object. This model is constructed by using the parameter(s) that achieved the maximum score and refitting the model to the complete data set.

```
gs.best_estimator_
```

```
Ridge(alpha=0.03290344562312668, fit_intercept=False)
```

```
gs.best_estimator_.coef_
```

```
array([ 0.99499,  2.00747,  0.00231, -3.0007 ,  0.49316,  0.10189, -0.29408,  1.00767])
```

```
gs.best_estimator_.predict(X)
```

```
array([ -0.12179,   3.34151,   0.76055,   7.89292,   1.56523,  -5.33575,  -4.37469,   3.13003,  -0.16859,  -
        -1.96548,   2.99039,   0.56796,  -5.26672,   5.4966 ,   3.47247,  -2.66117,   3.35011,   0.64221,  -
         0.76008,   5.49779,   2.6521 ,  -0.83127,   0.04167,  -1.92585,  -2.48865,   2.29127,   3.62514,  -
        -2.78598, -12.55143,   2.79189,  -1.89763,  -5.1769 ,   1.87484,   2.18345,  -6.45358,   0.91006,
         1.04564,  -1.54843,   0.76161,  -1.65495,   0.22378,  -0.68221,   0.12976,   2.58875,   2.54421,  -
         0.36935,   0.87397,   9.22348,  -1.29078,   1.74347,  -1.55169,  -0.69398,  -1.40445,   0.23072,
         1.70208,   7.15821,   3.96172,   5.75363,  -4.50718,  -5.81785,  -2.47424,   1.19276,   2.57431,  -
         2.65413,  -0.67486,  -3.01324,   0.34118,  -3.83856,   0.33096,  -3.59485,  -1.55578,   0.96765,
        -2.65588,  -5.77111,  -1.20292,   2.66903,  -1.11387,   3.05231,   6.34596,  -1.42886,  -2.29709,  -
         1.14603,  -3.35087,  -5.91052,  -1.23355,   2.8308 ,  -3.21438,   4.09019,  -5.95969,  -0.98044,
         2.67859,   2.45406,  -2.28901,   1.1609 ,  -1.50239,  -5.51199,   2.67089,   2.39878,   6.65249,
 -0.85644,   1.90162,  -1.23686,   3.22403,   5.31725,   0.31415,   0.17128,  -1.53623,   1.73354,  -
 -0.67864,  -0.67348,   4.22499,   3.34704,  -1.44927,  -6.3229 ,   4.83881,  -3.71184,   6.32207,
  5.69233,   6.28949,   5.37201,  -0.63177,   2.88795,   4.01781,   7.03453,   1.76797,   5.86793,
 -0.92299,  -4.85603,   4.18714,  -3.60775,  -2.31532,   1.27459,   0.37238,  -1.21   ,   2.44074,  -
  0.8058 ,   0.23748,   1.13615,   0.63385,  -0.2395 ,   6.07024,   0.85521,   0.18951,   3.27772,  -
-10.86754,  -9.25489,   7.0615 ,   0.01263,   3.93274,   3.40325,  -1.57858,  -4.94508,  -2.69779,
 -0.03725,  -1.15642,   8.92035,   2.63769,  -1.39664,   1.62241,  -4.87487,  -2.49769,   1.39569,  -
 -4.41299,  -4.79775,  -3.79204,  -3.61711,  -2.92489,   7.15104,  -3.24195,   3.03705,  -4.01473,  -
 10.77554,  -1.64465,  -2.13624,  -2.16392,   1.92049,  -2.47602,  -4.34462,  -2.09427,  -0.32466,
 -3.28827,  -5.73513,   4.76249,  -1.24714,   0.08253,  -1.71446,   1.3742 ,   1.85738,  -6.37864,  -
 -4.48298,  -0.28666,  -4.92509,   2.6523 ,  -4.59622,   3.09283,   3.50353,  -6.1787 ,  -2.08203,  -
```

`cv_results_` attribute

Other useful details about the grid search process are stored in the dictionary `cv_results_` attribute which includes things like average test scores, fold level test scores, test ranks, test runtimes, etc.

```python
gs.cv_results_.keys()
```

```
dict_keys(['mean_fit_time', 'std_fit_time', 'mean_score_time', 'std_score_time', 'param_alpha', 'params', 's
```

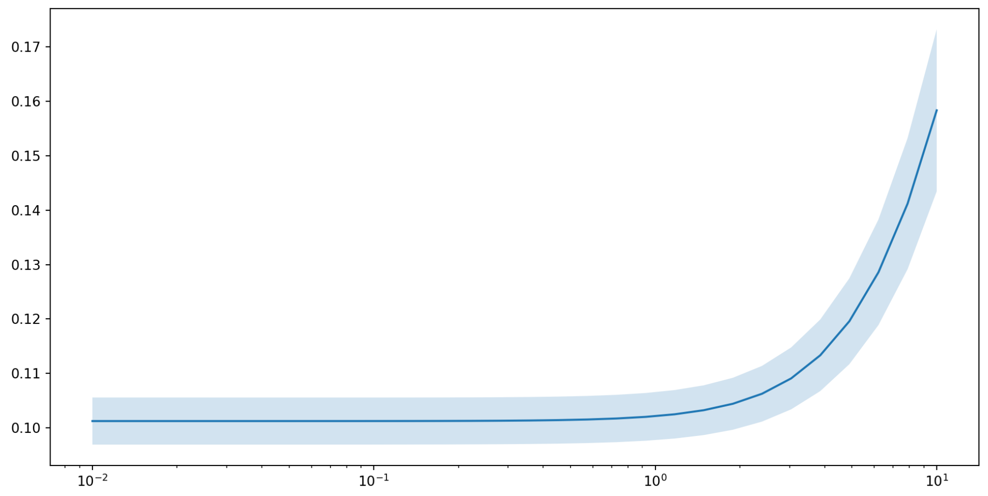
```python
gs.cv_results_["param_alpha"]
```

```
masked_array(data=[0.01, 0.01268961003167922, 0.01610262027560939, 0.020433597178569417, 0.02592943797404667
                   0.08531678524172806, 0.10826367338740546, 0.1373823795883263, 0.17433288221999882, 0.2212
                   0.5736152510448679, 0.727895384398315, 0.9236708571873861, 1.1721022975334805, 1.4873521(
                   4.893900918477494, 6.2101694189156165, 7.880462815669913, 10.0],
             mask=[False, False, False, False, False, False, False, False, False, False, False, False, False
                   False, False, False, False, False],
       fill_value='?',
            dtype=object)
```

```python
gs.cv_results_["mean_test_score"]
```

```
array([-0.10126, -0.10126, -0.10126, -0.10126, -0.10126, -0.10126, -0.10126, -0.10126, -0.10126, -0.10126, -
       -0.10203, -0.1025 , -0.10325, -0.10444, -0.10627, -0.10909, -0.11333, -0.11959, -0.12859, -0.14119, -
```

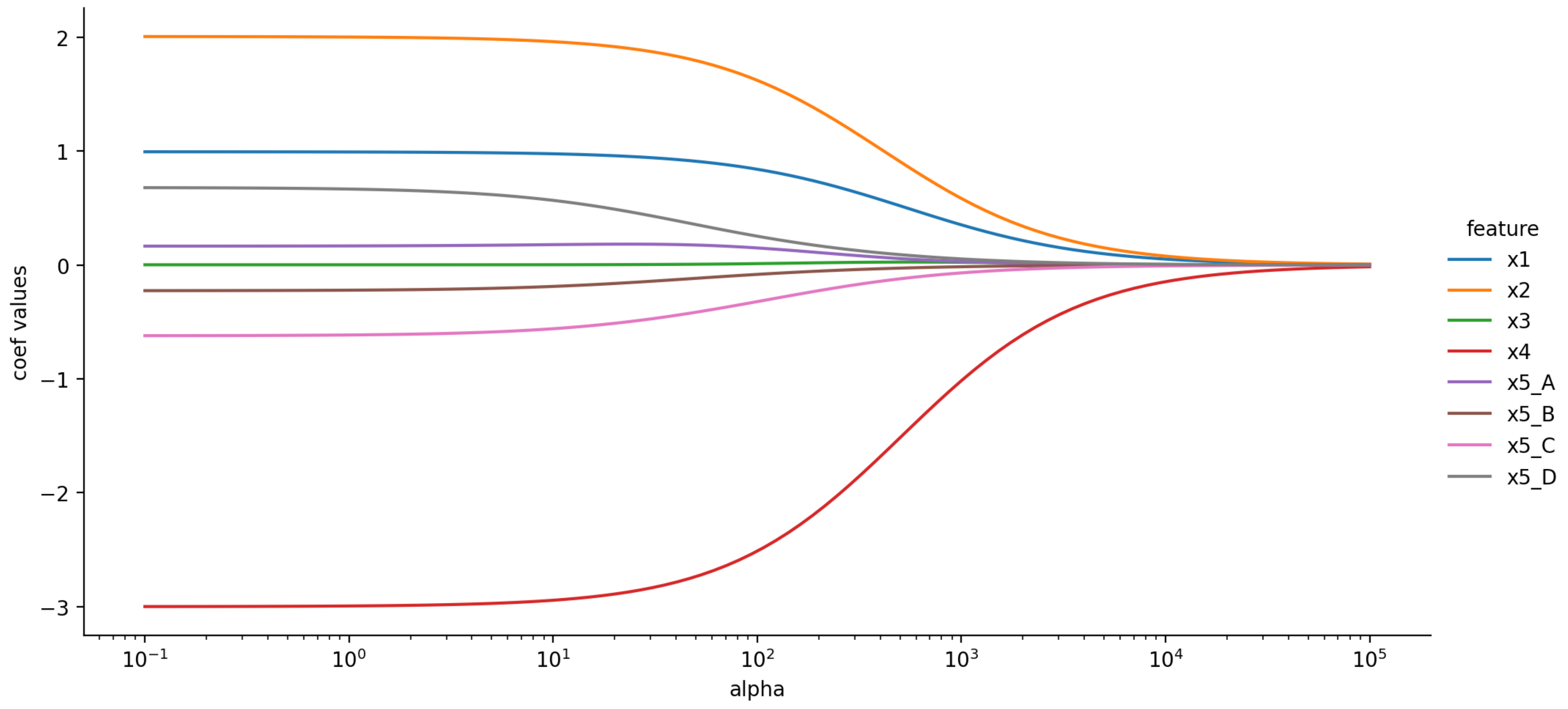
```python
alpha = np.array(gs.cv_results_["param_alpha"],d
score = -gs.cv_results_["mean_test_score"]
score_std = gs.cv_results_["std_test_score"]
n_folds = gs.cv.get_n_splits()

plt.figure(layout="constrained")

ax = sns.lineplot(x=alpha, y=score)
ax.set_xscale("log")

plt.fill_between(
  x = alpha,
  y1 = score + 1.96*score_std / np.sqrt(n_folds)
  y2 = score - 1.96*score_std / np.sqrt(n_folds)
  alpha = 0.2
)

plt.show()
```



Ridge traceplot

```
alpha = np.logspace(-1,5, 100)
betas = []

for a in alpha:
    rg = Ridge(alpha=a).fit(X, y)

    betas.append(rg.coef_)

res = pd.DataFrame(
  data = betas, columns = rg.feature_names_in_
).assign(
  alpha = alpha
)
```

```python
g = sns.relplot(
  data = res.melt(id_vars="alpha", value_name="coef values", var_name="feature"),
  x = "alpha", y = "coef values", hue = "feature",
  kind = "line", aspect=2
)
g.set(xscale="log")
```


coef values
alpha
10^{-1}
10^{0}
10^{1}
10^{2}
10^{3}
10^{4}
10^{5}
feature
x1
x2
x3
x4
x5_A
x5_B
x5_C
x5_D