Mud card answers

- **Since we already did splitting and preprocessing in step 2 and 3, then use the training set to choose ML models. When we fine tune the hyperparemeters of the models, does it mean we need to split and preprocess the whole data sets once again or just used the prepared sets from step 2 and 3.**
  - yes, you just use the prepared sets
- **"Can the SVR deal with the target variable with string? Because the randomforest model works properly with the y_train which is the house price but the SVR shows a wrong code that could not convert string to float: ' <=50K'**
  - SVR stands for Support Vector *Regression* so it won't work with the adult dataset's income target variable
  - use SVC - the Support Vector *Classifier*
- **"Why maximum feature is between 0 and 1 in this dataset? Is that proportion? 'max_features': [0.5,0.75,1.0] # linearly spaced between 0.5 and 1"**
  - yes, read through te manual
  - if max_features is a float, it is the proportion of features to use and it needs to be between 0 and 1
  - if max_features is an int, it's the number of features to use
- **Is the Kfold in GridSearchCV the same as the kfolds we implement to get different training, validation, and test sets? It looks like it. So then we would have to build another for-loop for each iteration of our datas kfolds?**
  - I'm not sure what implementation you are referring to, please come to the office hours
- **do we never process y?**
  - no, usually it's not necessary unless the regression variable is weirdly formatted
- **How is the train test split introduced into the GridSearchCV**
  - that's exactly what the last quiz of the previous lecture was about so check the solution on canvas
- **Why don't need to tune the kernel of SVC**
  - you could tune it
  - I focused mainly in the rbf kernel in class
- **I've seen Bayesian Optimization used for hyperparameter tuning of neural networks. Is this overkill for the techniques described in class given that there are much fewer parameters to tune?**
- **Do you have any books/resources that you recommend for more sophisticated grid search methods?**
  - sklearn doesn't support it but you can write code to try it
  - usually it's not worth the effort
  - a better hyperparameter tuning algorithm can only give a modest improvement on model performance
  - if you want to boost your model, generate new features
- **In most situation dealing with large (even with only 1000 images), GridSearchCV would cause out of RAM issues. At that time is hand-selecting and recording results**

the only option? Or there are still some automated ways to do those.
  - I'm not sure why GridSearchCV would run out of RAM with ~1000 images
  - any reasonable laptop nowadays should be able to handle that
  - maybe the problem is something else?

When the iid assumption breaks down

- What is the intended use of the model? What is it supposed to do/predict?
- What data do you have available at that time?
- Your cross validation must simulate the intended use of the model!

An example: seizure project

- you can read the publication here
- classification problem:
  - epileptic seizures vs. non-epileptic psychogenic seizures
- data from empatica wrist sensor
  - heart rate, skin temperature, EDA, blood volume pressure, acceleration
- data collection:
  - patients come to the hospital for a few days
  - eeg and video recording to determine seizure type
  - wrist sensor data is collected
- question:
  - Can we use the wrist sensor data to differentiate the two seizure types on new patients?

In [1]:

```
import pandas as pd
import numpy as np

df = pd.read_csv('data/seizure_data.csv')
print(df[df['patient ID'] == 32])
```

```
    patient ID           seizure_ID  ACC_mean  BVP_mean  EDA_mean    HR_mean  \
5           32  ID32__day3_arm_1_sz1  1.028539 -0.092102  0.112795  64.748167
6           32  ID32__day3_arm_1_sz1  1.027986  0.745437  0.130486  63.715667
7           32  ID32__day2_arm_1_sz0  1.002146  0.150810  0.189272  61.838500
8           32  ID32__day2_arm_1_sz0  1.005410  0.482859  1.226038  66.240833
9           32  ID32__day1_arm_1_sz0  0.997017 -0.925122  0.200990  56.103667
10          32  ID32__day1_arm_1_sz0  1.009207  1.618456  1.679754  64.668167
27          32  ID32__day1_arm_1_sz0  1.000290  0.046690  0.123165  54.289500
28          32  ID32__day1_arm_1_sz0  1.010351  0.125039  0.471180  65.060667
29          32  ID32__day2_arm_1_sz0  1.018163  0.254302  0.206010  61.875833
30          32  ID32__day2_arm_1_sz0  1.016785  1.242893  0.954649  66.216167
34          32  ID32__day3_arm_1_sz1  1.008867  0.070180  0.195966  65.995667
35          32  ID32__day3_arm_1_sz1  1.009554  0.222872  0.229909  63.871000
58          32  ID32__day3_arm_1_sz0  1.008873 -0.550857  0.177822  67.750833
79          32  ID32__day3_arm_1_sz0  1.026840  0.355953  0.205273  69.124667

    TEMP_mean  ACC_stdev  BVP_stdev  EDA_stdev  ...  BVP_50th  EDA_50th  \
5   36.944833   0.007469  36.486091   0.003905  ...     1.815  0.112710
6   36.676333   0.028190  84.964155   0.018598  ...     2.210  0.131921
```

```
7   38.600333   0.003747   64.194294   0.024278  ...     6.985  0.186026
8   39.296083   0.035257  165.665784   0.891139  ...     1.140  1.062333
9   34.656667   0.022648   77.013336   0.132008  ...     3.800  0.142159
10  34.678000   0.046047  146.515297   0.438236  ...     5.585  1.690537
27  38.467417   0.019826   51.176639   0.014530  ...     7.765  0.124259
28  38.448000   0.077142   61.205657   0.156170  ...     3.290  0.510114
29  37.681583   0.006805   40.982246   0.017099  ...     1.455  0.202632
30  37.979500   0.032493  219.277839   0.612229  ...    -5.785  1.028171
34  40.659458   0.021812   49.981175   0.013259  ...     3.480  0.198570
35  40.481333   0.048531   37.409681   0.031963  ...     0.695  0.228677
58  39.906667   0.021431   27.472002   0.003085  ...     1.955  0.178073
79  34.490167   0.008165   40.742936   0.003550  ...     3.090  0.206207

    HR_50th  TEMP_50th  ACC_75th  BVP_75th  EDA_75th  HR_75th  TEMP_75th  \
5    65.060      36.95  1.029947   16.3725  0.115591  65.8175     36.990
6    62.175      36.81  1.029947   21.1625  0.147611  66.2100     36.840
7    61.840      38.61  1.006085   43.8850  0.209086  61.9000     38.790
8    62.325      39.37  1.008872   49.4325  2.313129  71.0625     39.390
9    56.110      34.66  0.996821   35.2700  0.176739  56.6050     34.660
10   65.790      34.66  1.021497   70.4800  1.998868  67.7725     34.735
27   53.960      38.49  1.002073   39.8525  0.133226  54.7425     38.500
28   65.285      38.45  1.014302   25.4625  0.577047  69.4975     38.530
29   61.910      37.68  1.022811   29.2125  0.219282  61.9300     37.750
30   64.700      38.00  1.022811   65.5000  1.503002  69.5725     38.030
34   66.145      40.68  1.013700   13.1300  0.199852  67.0425     40.710
35   64.395      40.49  1.016106   12.9650  0.260383  65.9625     40.530
58   68.170      39.93  1.015264   17.8625  0.179354  68.5725     40.030
79   69.810      34.37  1.033260   13.4550  0.207488  70.0000     34.680

    label
5     0.0
6     0.0
7     0.0
8     0.0
9     0.0
10    0.0
27    0.0
28    0.0
29    0.0
30    0.0
34    0.0
35    0.0
58    0.0
79    0.0

[14 rows x 48 columns]
```

In [2]:

```python
y = df['label']
patient_ID = df['patient ID']
seizure_ID = df['seizure_ID']
X = df.drop(columns=['patient ID','seizure_ID','label'])
classes, counts = np.unique(y,return_counts=True)
print('balance:',np.max(counts/len(y)))
```

```
balance: 0.6884057971014492
```

In [3]:

```python
from sklearn.svm import SVC
from sklearn.metrics import accuracy_score
from sklearn.model_selection import StratifiedKFold
from sklearn.model_selection import train_test_split
```

```
from sklearn.preprocessing import StandardScaler
from sklearn.pipeline import make_pipeline
from sklearn.model_selection import KFold
from sklearn.model_selection import GridSearchCV
from sklearn.metrics import make_scorer

def ML_pipeline_kfold_GridSearchCV(X,y,random_state,n_folds):
    # create a test set
    X_other, X_test, y_other, y_test = train_test_split(X, y, test_size=0.2, ran
    # splitter for _other
    kf = StratifiedKFold(n_splits=n_folds,shuffle=True,random_state=random_state
    # create the pipeline: preprocessor + supervised ML method
    scaler = StandardScaler()
    pipe = make_pipeline(scaler,SVC())
    # the parameter(s) we want to tune
    param_grid = {'svc__C': np.logspace(-3,4,num=8),'svc__gamma': np.logspace(-3
    # prepare gridsearch
    grid = GridSearchCV(pipe, param_grid=param_grid,scoring = make_scorer(accura
                        cv=kf, return_train_score = True)
    # do kfold CV on _other
    grid.fit(X_other, y_other)
    return grid, grid.score(X_test, y_test)
```

In [4]:

```
test_scores = []
for i in range(5):
    grid, test_score = ML_pipeline_kfold_GridSearchCV(X,y,i*42,5)
    print(grid.best_params_)
    print('best CV score:',grid.best_score_)
    print('test score:',test_score)
    test_scores.append(test_score)
print('test accuracy:',np.around(np.mean(test_scores),2),'+/-',np.around(np.std(
```

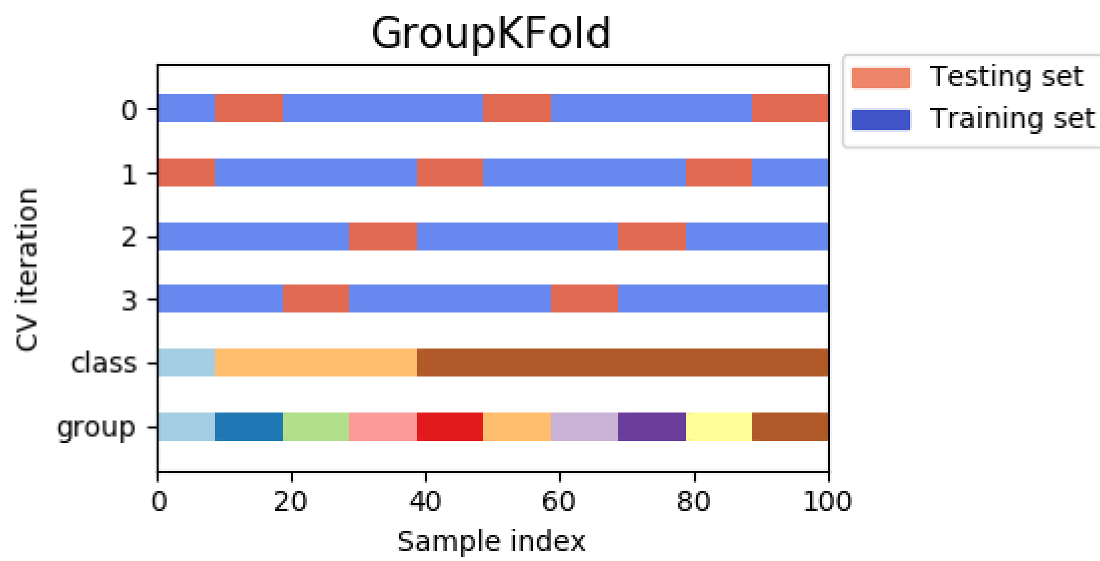
```
{'svc__C': 1.0, 'svc__gamma': 0.01}
best CV score: 0.9227272727272726
test score: 0.9285714285714286
{'svc__C': 10.0, 'svc__gamma': 0.01}
best CV score: 0.9363636363636363
test score: 0.9285714285714286
{'svc__C': 10.0, 'svc__gamma': 0.01}
best CV score: 0.9045454545454547
test score: 0.9464285714285714
{'svc__C': 10.0, 'svc__gamma': 0.01}
best CV score: 0.9
test score: 0.9285714285714286
{'svc__C': 10.0, 'svc__gamma': 0.01}
best CV score: 0.9363636363636363
test score: 0.9107142857142857
test accuracy: 0.93 +/- 0.01
```

This is wrong! A very bad case of data leakage!

- the textbook case of information leakage!
- if we just do KFold CV blindly, the points from the same patient end up in different sets
    - when you deploy the model and apply it to data from new patients, that patient's data will be seen for the first time
- the ML pipeline needs to mimic the intended use of the model!

- we want to split the points based on the patient ID!
- we want all points from the same patient to be in either train/CV/test

Group-based split: GroupKFold



In [5]:

```
from sklearn.model_selection import GroupKFold
from sklearn.model_selection import GroupShuffleSplit
def ML_pipeline_groups_GridSearchCV(X,y,groups,random_state,n_folds):
    # create a test set based on groups
    splitter = GroupShuffleSplit(n_splits=1,test_size=0.2,random_state=random_st
    for i_other,i_test in splitter.split(X, y, groups):
        X_other, y_other, groups_other = X.iloc[i_other], y.iloc[i_other], group
        X_test, y_test, groups_test = X.iloc[i_test], y.iloc[i_test], groups.ilo
    # check the split
#     print(pd.unique(groups))
#     print(pd.unique(groups_other))
#     print(pd.unique(groups_test))
    # splitter for _other
    kf = GroupKFold(n_splits=n_folds)
    # create the pipeline: preprocessor + supervised ML method
    scaler = StandardScaler()
    pipe = make_pipeline(scaler,SVC())
    # the parameter(s) we want to tune
    param_grid = {'svc__C': np.logspace(-3,4,num=8),'svc__gamma': np.logspace(-3
    # prepare gridsearch
    grid = GridSearchCV(pipe, param_grid=param_grid,scoring = make_scorer(accura
                        cv=kf, return_train_score = True)
    # do kfold CV on _other
    grid.fit(X_other, y_other, groups=groups_other)
    return grid, grid.score(X_test, y_test)
```

In [6]:

```
test_scores = []
for i in range(5):
    grid, test_score = ML_pipeline_groups_GridSearchCV(X,y,patient_ID,i*42,5)
    print(grid.best_params_)
    print('best CV score:',grid.best_score_)
    print('test score:',test_score)
```

```
    test_scores.append(test_score)
print('test accuracy:',np.around(np.mean(test_scores),2),'+/-',np.around(np.std(
```

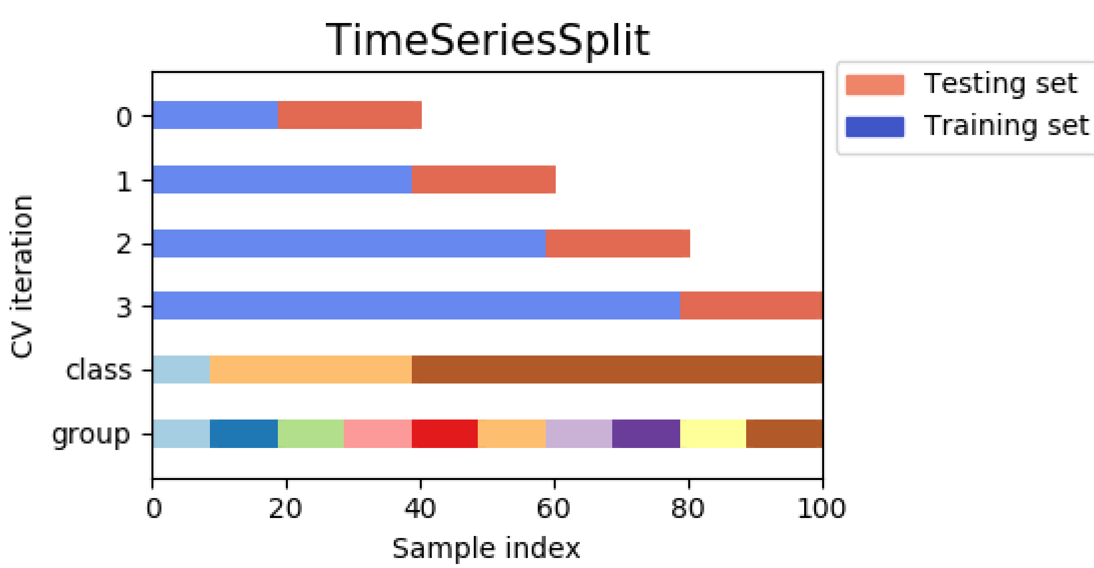
```
{'svc__C': 10.0, 'svc__gamma': 0.001}
best CV score: 0.7609139784946237
test score: 0.6410256410256411
{'svc__C': 0.1, 'svc__gamma': 0.01}
best CV score: 0.6522727272727272
test score: 0.2711864406779661
{'svc__C': 10.0, 'svc__gamma': 0.001}
best CV score: 0.5720073891625616
test score: 0.9390243902439024
{'svc__C': 10.0, 'svc__gamma': 0.001}
best CV score: 0.7061742424242425
test score: 0.43243243243243246
{'svc__C': 10000.0, 'svc__gamma': 0.001}
best CV score: 0.6082407407407406
test score: 0.8901098901098901
test accuracy: 0.63 +/- 0.26
```

The takeaway

- an incorrect cross validation pipeline gives misleading results
    - usually the model appears to be pretty accurate
    - but the performance is poor when the model is deployed
- this can be avoided by a careful cross validation pipeline
    - think about how your model will be used
    - mimic that future use in CV

Data leakage in time series data is similar!

- do NOT use information in CV which will not be available once your model is deployed
    - don't use future information!



Time series data

- stock price, crypto price, covid-19 positive case counts, etc
- simple data structure:

time	observation
t_0	y_0
t_1	y_1
t_2	y_2
...	...
t_i	y_i
...	...
t_n-1	y_n-1
t_n	y_n

- assumption:
  - the difference between two time points (dt) is constant
  - e.g., 1 minute, 5 minutes, 1 hour, or 1 day

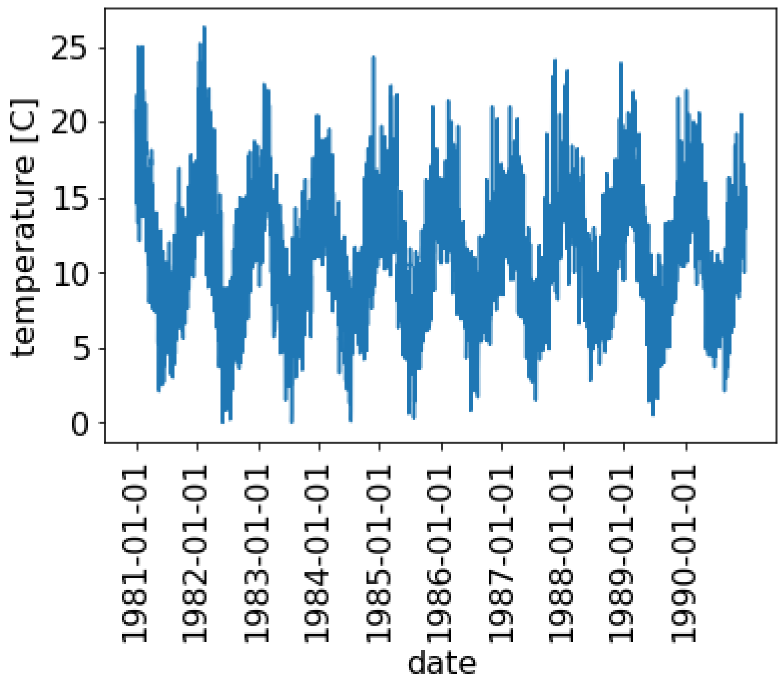
Autocorrelation

- the correlation of the time series data with a delayed copy of itself
- delay on the x axis, correlation coefficient on the y axis
- if delay = 0, the correlation coefficient is 1
- if the delay is short, autocorrelation can be high
- autocorrelation tends to subside for longer delays
- let's check an example

In [8]:

```
import pandas as pd
import matplotlib.pyplot as plt
import matplotlib
import numpy as np
matplotlib.rcParams.update({'font.size': 16})

df = pd.read_csv('data/daily-min-temperatures.csv')
print(df.shape)
print(df.head())

plt.plot(df['Temp'])
plt.xticks(np.arange(len(df['Date']))[::365],df['Date'].iloc[::365],rotation=90)
plt.xlabel('date')
plt.ylabel('temperature [C]')
plt.show()
```

```
(3650, 2)
         Date  Temp
0  1981-01-01  20.7
1  1981-01-02  17.9
2  1981-01-03  18.8
3  1981-01-04  14.6
4  1981-01-05  15.8
```

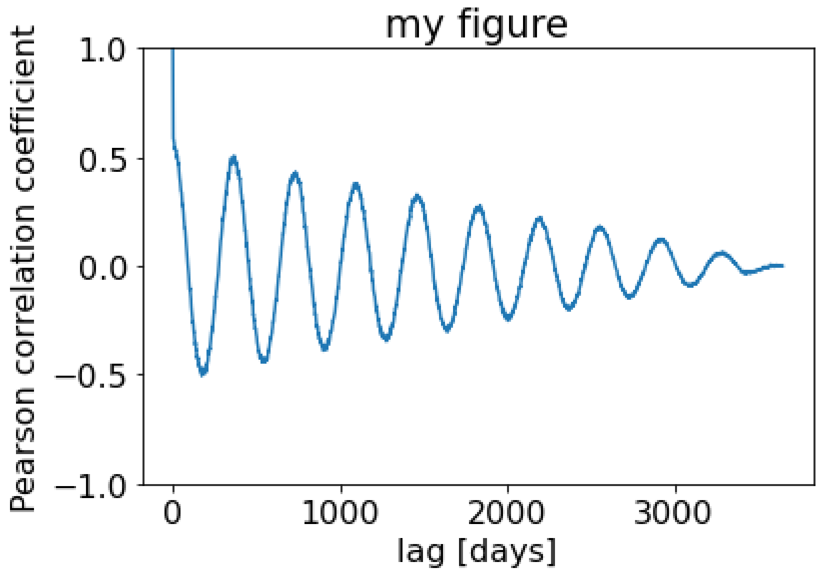


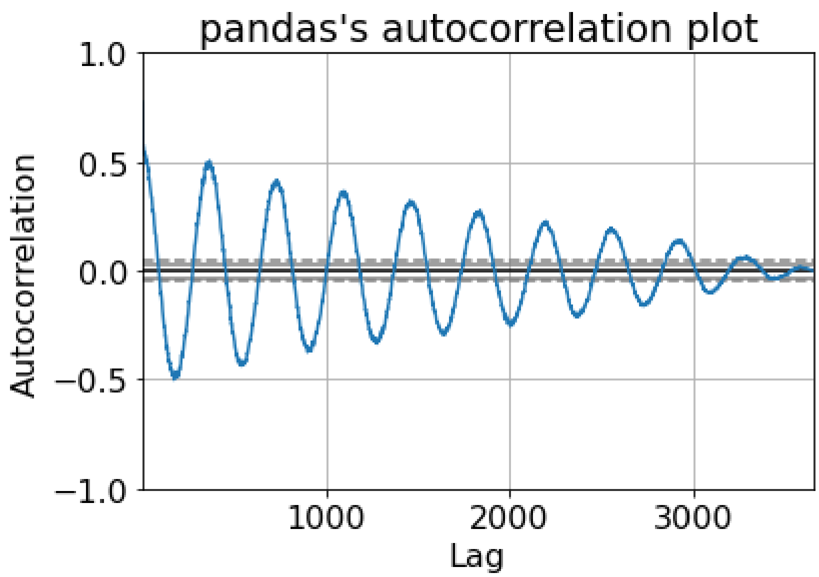
In [9]:

```
# let's create an autocorrelation plot

lags = np.arange(3650)
corr_coefs = np.zeros(3650)

for i in np.arange(len(lags)):
    x = df['Temp'].iloc[i:-1].reset_index(drop=True) # recent observations
    y = df['Temp'].iloc[:-i-1].reset_index(drop=True) # lag-shifted observations
    # the shapes must be the same
    if x.shape != y.shape:
        raise ValueError('shape mismatch!')
    # Pearson correlation multiplied by the fraction of time series used
    corr_coefs[i] = x.corr(y,method='pearson')*x.shape[0]/df['Temp'].shape[0]
print(corr_coefs[:10])

plt.plot(lags,corr_coefs)
plt.ylim([-1,1])
plt.xlabel('lag [days]')
plt.ylabel('Pearson correlation coefficient')
plt.title('my figure')
plt.show()

# a one-liner
pd.plotting.autocorrelation_plot(df['Temp'])
plt.title("pandas's autocorrelation plot")
plt.show()
```

```
[0.99972603 0.77446147 0.63057611 0.58570362 0.5780733  0.57758888
 0.57542059 0.57472479 0.56812066 0.56190417]
```

```
/Users/azsom/opt/anaconda3/envs/data1030/lib/python3.9/site-packages/numpy/lib/f
unction_base.py:2683: RuntimeWarning: Degrees of freedom <= 0 for slice
  c = cov(x, y, rowvar, dtype=dtype)
/Users/azsom/opt/anaconda3/envs/data1030/lib/python3.9/site-packages/numpy/lib/f
unction_base.py:2542: RuntimeWarning: divide by zero encountered in true_divide
  c *= np.true_divide(1, fact)
```





Autoregression: create an iid feature matrix using lag features

- goal:
    - predict what y will be dt in the future
- the target variable and lag features:

feature_1	feature_2	...	feature_m-1	feature m	target variable
y_0	y_1	...	y_m-1	y_m	y_m+1
y_1	y_2	...	y_m	y_m+1	y_m+2
...	...	...	...	...	...
y_i-m	y_i-m+1	...	y_i-2	y_i-1	y_i
...	...	...	...	...	...
y_n-m	y_n-m+1	...	y_n-2	y_n-1	y_n

- the features are shifted with respect to the original observation with a dt lag
- this feature matrix is now iid and can be split with any of the methods we covered in the previous lecture

In [10]:

```
y = df['Temp']
X = pd.concat([df['Temp'].shift(3),df['Temp'].shift(2),df['Temp'].shift(1)],axis
X.columns = ['lag 3 days','lag 2 days','lag 1 day']
print(X.tail(10))
print(y.tail(10))
```

```
      lag 3 days  lag 2 days  lag 1 day
3640        14.7        15.4       13.1
3641        15.4        13.1       13.2
3642        13.1        13.2       13.9
3643        13.2        13.9       10.0
3644        13.9        10.0       12.9
3645        10.0        12.9       14.6
3646        12.9        14.6       14.0
3647        14.6        14.0       13.6
3648        14.0        13.6       13.5
3649        13.6        13.5       15.7
3640    13.2
3641    13.9
3642    10.0
3643    12.9
3644    14.6
3645    14.0
3646    13.6
3647    13.5
3648    15.7
3649    13.0
Name: Temp, dtype: float64
```

Things to consider

- lag between the target variable and feature m can be more if you want to predict the observation multiple dt's in the future
- you might also have multiple time series to work with (prices of multiple stock, covid cases in multiple countries, etc)
    - all of those need to be shifted by the same lag relative to the target variable
- due to autocorrelation, the features closer in time to the target variable tend to be more predictive
- how many features should you use?
    - treat the number of features as a hyperparameter

Special scenarios

- what if dt is not consant and/or each time series have its own non-uniform time?
    - for example you try to predict crypto prices based on stock prices
        - stock prices are available once per hour
        - crypto prices are only available when a trade happens (i.e., some tokens are traded rarely)

- interpolate to a uniform time grid
    - try linear and non-linear interpolation techniques to figure out what works best
    - check out scipy for more info
    - cubic spline interpolation usually works well
- you might have a mix of time series and non-time series features
    - cvs customer purchase history
        - you know what a customer bought and when - time series part
        - you have info on the customer (gender, race, address, etc) - non-time series part

Mud card

In [ ]:
```

```