

Mudcard

- **Are there quantitative ways to determine how well the iid assumption holds on data?**
 - [here](#) is a good read on the topic
 - short answer is no
- **Following up to the discussion on sklearn's lack of support for support stratification where y is continuous: can you provide some insight on why (or what kind of cases) stratification would be necessary in a regression problem?**
 - PS4, problem 1c will cover this
 - it is a good idea to stratify, if the distribution of the regression target variable is heavy-tailed (e.g., exponential, log-normal)
 - if you do not stratify, some of your sets might not contain rare values from the heavy tail thus throwing off the regression model
- **In k-fold cross validation, will it make the model better if we shuffle the training/validation data before each round of training, instead of just shuffling once before taking k non-overlapping folds?**
 - that's not kfold, it's much closer to the basic split (train/validation/test)
- **If we want to predict a continuous variable, y, are imbalanced features still a concern?**
 - we don't really care about features being imbalanced
 - imbalance is important for a classification target variable
- **I am still confused on how the stratified K fold is implemented. Is it the same process regardless of the dataset we use?**
 - yes, these splitting strategies are independent of the dataset
 - the only constraint is that the dataset needs to be IID if you want to use kfold splitting
- **A bit confused why we would want to use KFold and cross-validation as opposed to normal splitting**
 - both are equally good as long as your dataset is IID
 - use whichever you prefer in your project
 - kfold is quite often used so I wanted you to be familiar with it
- **Why do we see different random states in different models? Example - on Kaggle, we see random state = 0/10/42, etc. Apart from splitting up the dataset into different points, does the value of the random state affect the data in any other way?**
 - you will see that some ML algorithms are non-deterministic (all decision tree-based models) and you'll need a random state for those otherwise your model changes every time you rerun the cell
- **To be clear: shuffling is just randomizing the index/order of the raw data?**
 - yep, randomly rearranges the rows

- **are test_size and train_size in the split methods pretty much specifying the same thing? I.e. does a test_size of 0.2 imply train_size 0.8?**
 - not the same thing
 - $\text{train_size} = 1 - \text{test_size}$
 - $\text{train_size} \neq \text{test_size}$ unless you want a 50-50 split
- **When using Kfold with 5 folds, should we still test the model on 10 different random states? So essentially we would be testing 50 different models?**
 - yes, that's recommended because if you use 5 folds once, that's still only one test score
- **What does this part of the k-fold splitting code mean: "for train_index, val_index in kf.split(X_other, y_other)"?**
 - print out train_index and val_index to check
- **Still a bit unclear about how stratification intuitively balances out unbalanced data sets. Just from a visualization standpoint.**
- **Can we apply stratify to balance datasets?**
 - stratification does NOT balance out an imbalanced dataset
 - if 1% of points belong to the minority class, stratification guarantees that all sets in your dataset will contain exactly 1% of the minority class
- **If train_test_split randomly separates the dataset already, why do we still need a shuffle argument for the function?**
 - experiment with the code below to figure it out

```
from sklearn.model_selection import train_test_split
import numpy as np
X, y = np.arange(20).reshape((10, 2)), range(10)
print(X, y)
```

```
X_train, X_test, y_train, y_test = train_test_split(X, y,
test_size=0.33, random_state=42, shuffle=False)
```

```
print(y_train, y_test)
```

- **could you specify why is random walk sequence not iid?**
 - D the underlying distribution changes as soon as a step is taken
- **I want to know when should I use KFold and when can use simple train-val-test split.**
 - both are equally good if your dataset is IID
- **The baseline metric for regression was said in class to be RMSE. How is the baseline calculated?**
 - no, RMSE is not a baseline metric
 - RMSE is one metric you can use with regression datasets
 - the baseline RMSE of a regression problem can be determined if you calculate the RMSE with respect to the mean of the target variable
 - we will cover this in a few weeks
- **I understand that KFold splits for us but what exactly are we testing for, what is the test? is it a test of balance or just whatever test we code?**

- you want to have a test set to calculate the generalization error
- **I am curious about the arguments in function, should we remember arguments or look for specific arguments using help function when we need it? How is the situation when having this kind of interview?**
 - I still look up arguments all the time :)
 - some arguments stick if you use them often enough (like stratify, random_state, some plotting arguments)
 - you are not expected to know all arguments of sklearn, numpy, or pandas methods during an interview

Split non-iid data

By the end of this lecture, you will be able to

- split non-iid data based on group ID
- split non-iid time series data

The supervised ML pipeline

The goal: Use the training data (X and y) to develop a **model** which can **accurately** predict the target variable (y_new) for previously unseen data (X_new).

1. Exploratory Data Analysis (EDA): you need to understand your data and verify that it doesn't contain errors

- do as much EDA as you can!

2. Split the data into different sets: most often the sets are train, validation, and test (or holdout)

- practitioners often make errors in this step!
- you can split the data randomly, based on groups, based on time, or any other non-standard way if necessary to answer your ML question

3. Preprocess the data: ML models only work if X and Y are numbers! Some ML models additionally require each feature to have 0 mean and 1 standard deviation (standardized features)

- often the original features you get contain strings (for example a gender feature would contain 'male', 'female', 'non-binary', 'unknown') which needs to be transformed into numbers
- often the features are not standardized (e.g., age is between 0 and 100) but it needs to be standardized

4. Choose an evaluation metric: depends on the priorities of the stakeholders

- often requires quite a bit of thinking and ethical considerations

5. Choose one or more ML techniques: it is highly recommended that you try multiple models

- start with simple models like linear or logistic regression
- try also more complex models like nearest neighbors, support vector machines, random forest, etc.

6. Tune the hyperparameters of your ML models (aka cross-validation)

- ML techniques have hyperparameters that you need to optimize to achieve best performance
- for each ML model, decide which parameters to tune and what values to try
- loop through each parameter combination
 - train one model for each parameter combination
 - evaluate how well the model performs on the validation set
- take the parameter combo that gives the best validation score
- evaluate that model on the test set to report how well the model is expected to perform on previously unseen data

7. Interpret your model: black boxes are often not useful

- check if your model uses features that make sense (excellent tool for debugging)
- often model predictions are not enough, you need to be able to explain how the model arrived to a particular prediction (e.g., in health care)

Examples of non-iid data

- if there is any sort of time or group structure in your data, it is likely non-iid
 - **group structure:**
 - **samples are not identically distributed, D might be different for each group**
 - a person appears multiple times in the dataset (e.g., hospital/doctor visits)
 - data is collected on multiple instruments (e.g., equipment failure prediction)
 - **time series data**
 - **values are not independent**
 - stocks price
 - covid19 cases
 - weather data

Ask yourself these questions!

- What is the intended use of the model? What is it supposed to do/predict?
- What data do you have available at the time of prediction?

- Your split must mimic the intended use of the model only then will you accurately estimate how well the model will perform on previously unseen points (generalization error).
- two examples:
 - if you want to predict the outcome of a new patient's visit to the ER:
 - your test score must be based on patients not included in training and validation
 - your validation score must be based on patients not included in training
 - points of one patient should not be distributed over multiple sets because your generalization error will be off
 - a youtube video was released 4 weeks ago and you want to predict if it will be featured a week from now, your training data should only contain info that will be available upon predictions (stuff you know 4 weeks after release)
 - split data based on youtube vid ID
 - use info that's available 4 weeks after release
 - your classification label will be whether it was featured or not 5 weeks after release

Split non-iid data

By the end of this lecture, you will be able to

- **split non-iid data based on group ID**
- split non-iid time series data

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]: 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]: 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, ra
    # splitter for _other
    kf = StratifiedKFold(n_splits=n_folds, shuffle=True, random_state=random_stat
    # 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(-
    # prepare gridsearch
    grid = GridSearchCV(pipe, param_grid=param_grid, scoring = make_scorer(accur
    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.stc
```

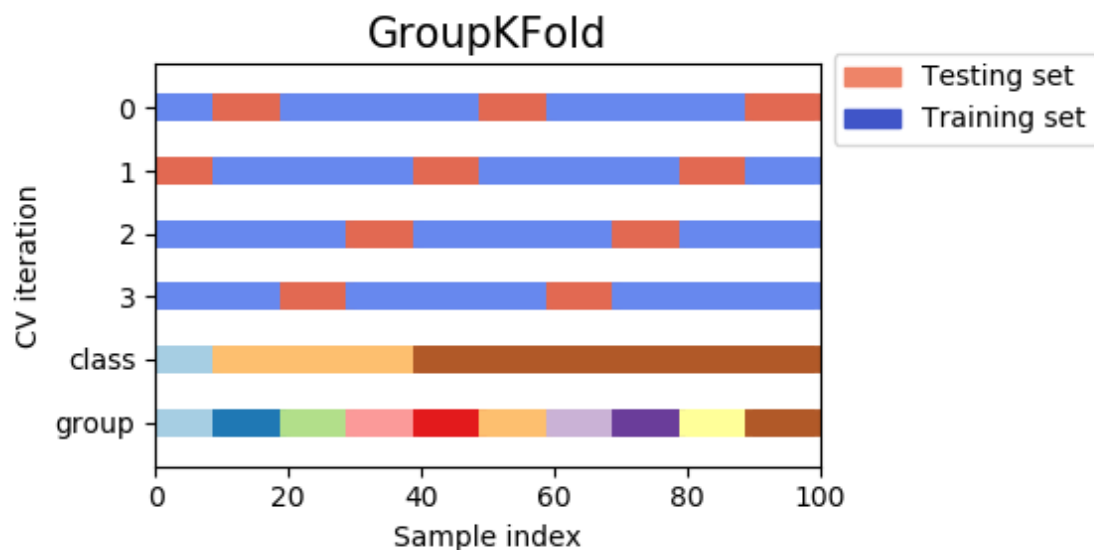


```
{'svc__C': 1.0, 'svc__gamma': 0.01}
best CV score: 0.9227272727272726
test score: 0.9285714285714286
{'svc__C': 10.0, 'svc__gamma': 0.01}
best CV score: 0.9363636363636363
test score: 0.9285714285714286
{'svc__C': 10.0, 'svc__gamma': 0.01}
best CV score: 0.9045454545454547
test score: 0.9464285714285714
{'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_s
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], grou
    X_test, y_test, groups_test = X.iloc[i_test], y.iloc[i_test], groups.il
# 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(-
# prepare gridsearch
grid = GridSearchCV(pipe, param_grid=param_grid, scoring = make_scorer(accur
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.stc

```

```

{'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

```

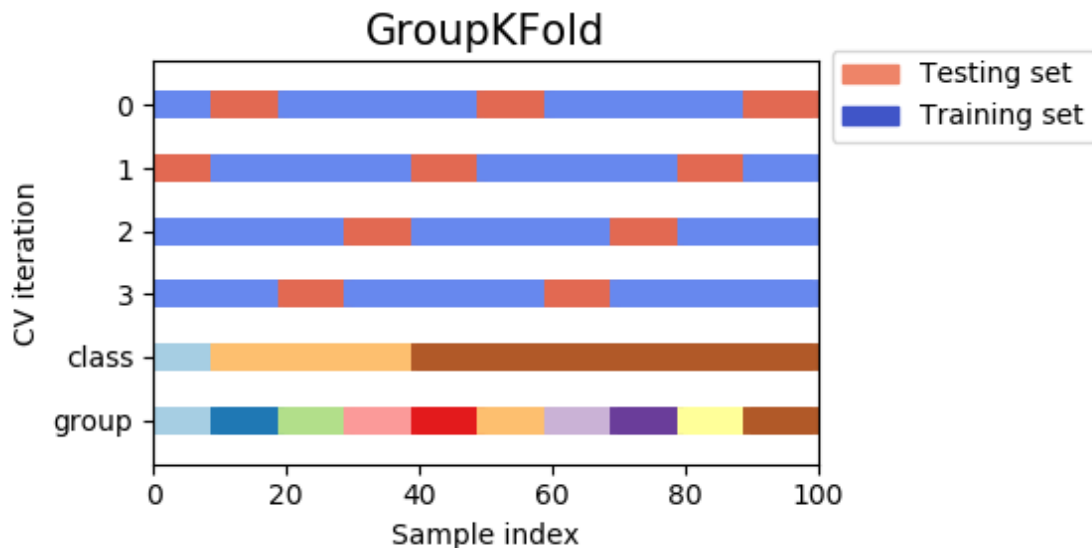
The takeaway

- 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

Let's take a look at group splitters using toy datasets

Group-based split: GroupKFold



```
In [7]: from sklearn.model_selection import GroupKFold
import numpy as np

X = np.ones(shape=(8, 2))
y = np.ones(shape=(8, 1))
groups = np.array([1, 1, 2, 2, 2, 3, 3, 3])

group_kfold = GroupKFold(n_splits=3)

for train_index, test_index in group_kfold.split(X, y, groups):
    print("TRAIN:", train_index, "TEST:", test_index)

TRAIN: [0 1 2 3 4] TEST: [5 6 7]
TRAIN: [0 1 5 6 7] TEST: [2 3 4]
TRAIN: [2 3 4 5 6 7] TEST: [0 1]
```

```
In [8]: help(GroupKFold)
```

Help on class GroupKFold in module sklearn.model_selection._split:

```
class GroupKFold(_BaseKFold)
```

```
    GroupKFold(n_splits=5)
```

K-fold iterator variant with non-overlapping groups.

The same group will not appear in two different folds (the number of distinct groups has to be at least equal to the number of folds).

The folds are approximately balanced in the sense that the number of distinct groups is approximately the same in each fold.

Read more in the :ref:`User Guide <group_k_fold>`.

Parameters

`n_splits` : int, default=5

Number of folds. Must be at least 2.

.. versionchanged:: 0.22

`n_splits` default value changed from 3 to 5.`

Notes

Groups appear in an arbitrary order throughout the folds.

Examples

```
>>> import numpy as np
>>> from sklearn.model_selection import GroupKFold
>>> X = np.array([[1, 2], [3, 4], [5, 6], [7, 8]])
>>> y = np.array([1, 2, 3, 4])
>>> groups = np.array([0, 0, 2, 2])
>>> group_kfold = GroupKFold(n_splits=2)
>>> group_kfold.get_n_splits(X, y, groups)
2
>>> print(group_kfold)
GroupKFold(n_splits=2)
>>> for train_index, test_index in group_kfold.split(X, y, groups):
...     print("TRAIN:", train_index, "TEST:", test_index)
...     X_train, X_test = X[train_index], X[test_index]
...     y_train, y_test = y[train_index], y[test_index]
...     print(X_train, X_test, y_train, y_test)
...
TRAIN: [0 1] TEST: [2 3]
[[1 2]
 [3 4]] [[5 6]
 [7 8]] [1 2] [3 4]
TRAIN: [2 3] TEST: [0 1]
[[5 6]
 [7 8]] [[1 2]
 [3 4]] [3 4] [1 2]
```

See Also

`LeaveOneGroupOut` : For splitting the data according to explicit

domain-specific stratification of the dataset.

Method resolution order:

GroupKFold
_BaseKFold
BaseCrossValidator
builtins.object

Methods defined here:

`__init__(self, n_splits=5)`
Initialize self. See help(type(self)) for accurate signature.

`split(self, X, y=None, groups=None)`
Generate indices to split data into training and test set.

Parameters

`X` : array-like of shape (n_samples, n_features)
Training data, where `n_samples` is the number of samples
and `n_features` is the number of features.

`y` : array-like of shape (n_samples,), default=None
The target variable for supervised learning problems.

`groups` : array-like of shape (n_samples,)
Group labels for the samples used while splitting the dataset into
train/test set.

Yields

`train` : ndarray
The training set indices for that split.

`test` : ndarray
The testing set indices for that split.

Data and other attributes defined here:

`__abstractmethods__` = frozenset()

Methods inherited from `_BaseKFold`:

`get_n_splits(self, X=None, y=None, groups=None)`
Returns the number of splitting iterations in the cross-validator

Parameters

`X` : object
Always ignored, exists for compatibility.

`y` : object
Always ignored, exists for compatibility.

`groups` : object

Always ignored, exists for compatibility.

Returns

`n_splits : int`

Returns the number of splitting iterations in the cross-validator.

Methods inherited from `BaseCrossValidator`:

`__repr__(self)`

Return `repr(self)`.

Data descriptors inherited from `BaseCrossValidator`:

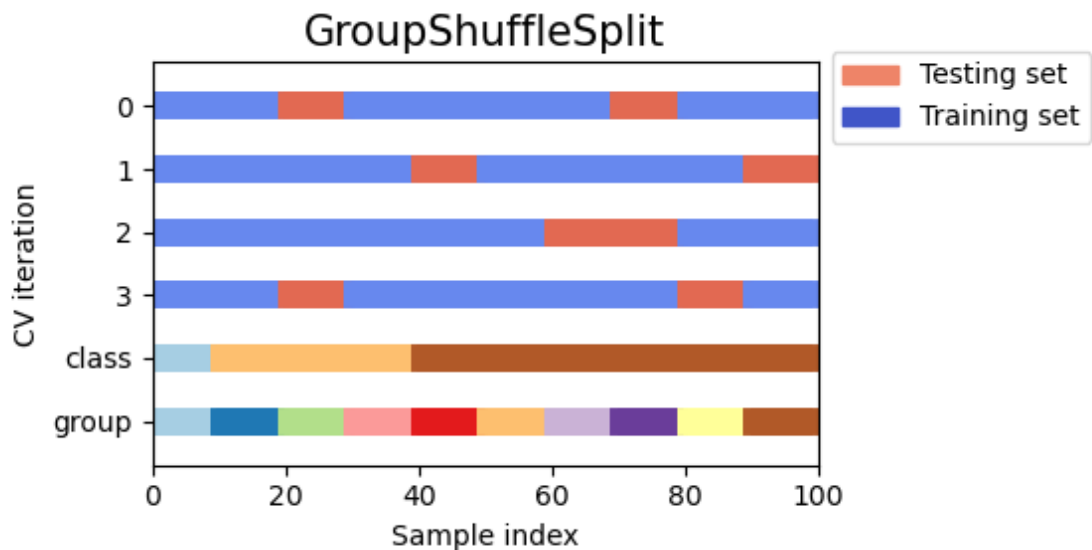
`__dict__`

dictionary for instance variables (if defined)

`__weakref__`

list of weak references to the object (if defined)

Group-based split: `GroupShuffleSplit`



```
In [9]: from sklearn.model_selection import GroupShuffleSplit

gss = GroupShuffleSplit(n_splits=5, train_size=.8, random_state=42)

for train_idx, test_idx in gss.split(X, y, groups):
    print("TRAIN:", train_idx, "TEST:", test_idx)
```

```
TRAIN: [2 3 4 5 6 7] TEST: [0 1]
TRAIN: [0 1 5 6 7] TEST: [2 3 4]
TRAIN: [2 3 4 5 6 7] TEST: [0 1]
TRAIN: [0 1 5 6 7] TEST: [2 3 4]
TRAIN: [2 3 4 5 6 7] TEST: [0 1]
```

Quiz 1

Go back to the GroupKFold example above. What happens when you change `n_splits` to 4? Why?

Why could we set the `n_splits` argument to 5 in `GroupShuffleSplit`? Check the manual of both methods to find the answer.

Explain your answer in a couple of sentences!

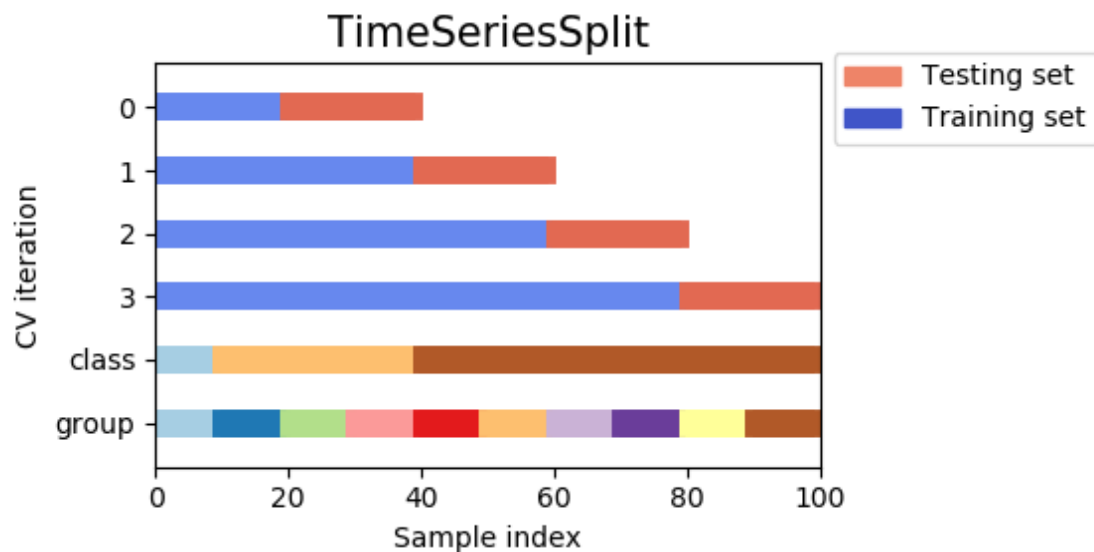
Split non-iid data

By the end of this lecture, you will be able to

- split non-iid data based on group ID
- **split non-iid time series data**

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

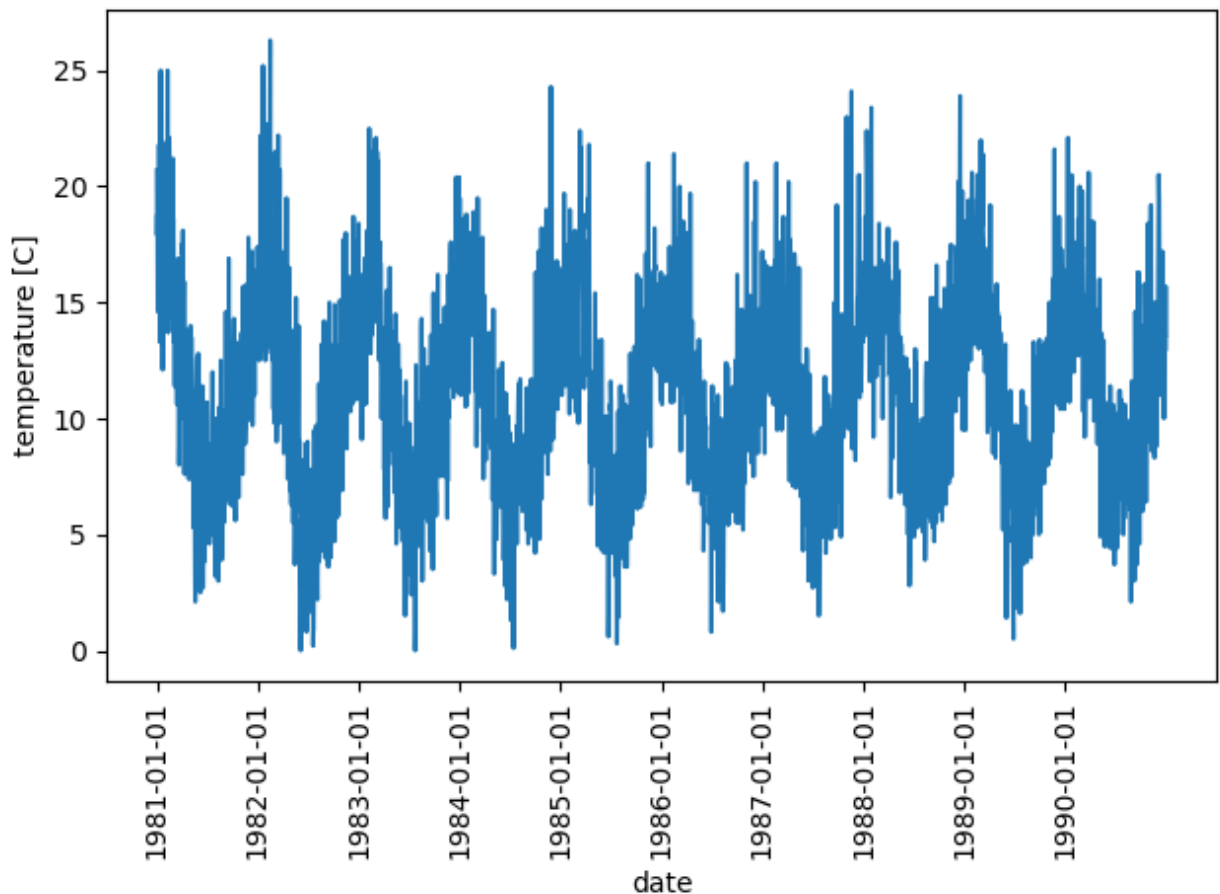
```
In [10]: import pandas as pd
import matplotlib.pyplot as plt
import matplotlib
import numpy as np

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.tight_layout()
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 [11]: # let's create an autocorrelation plot

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

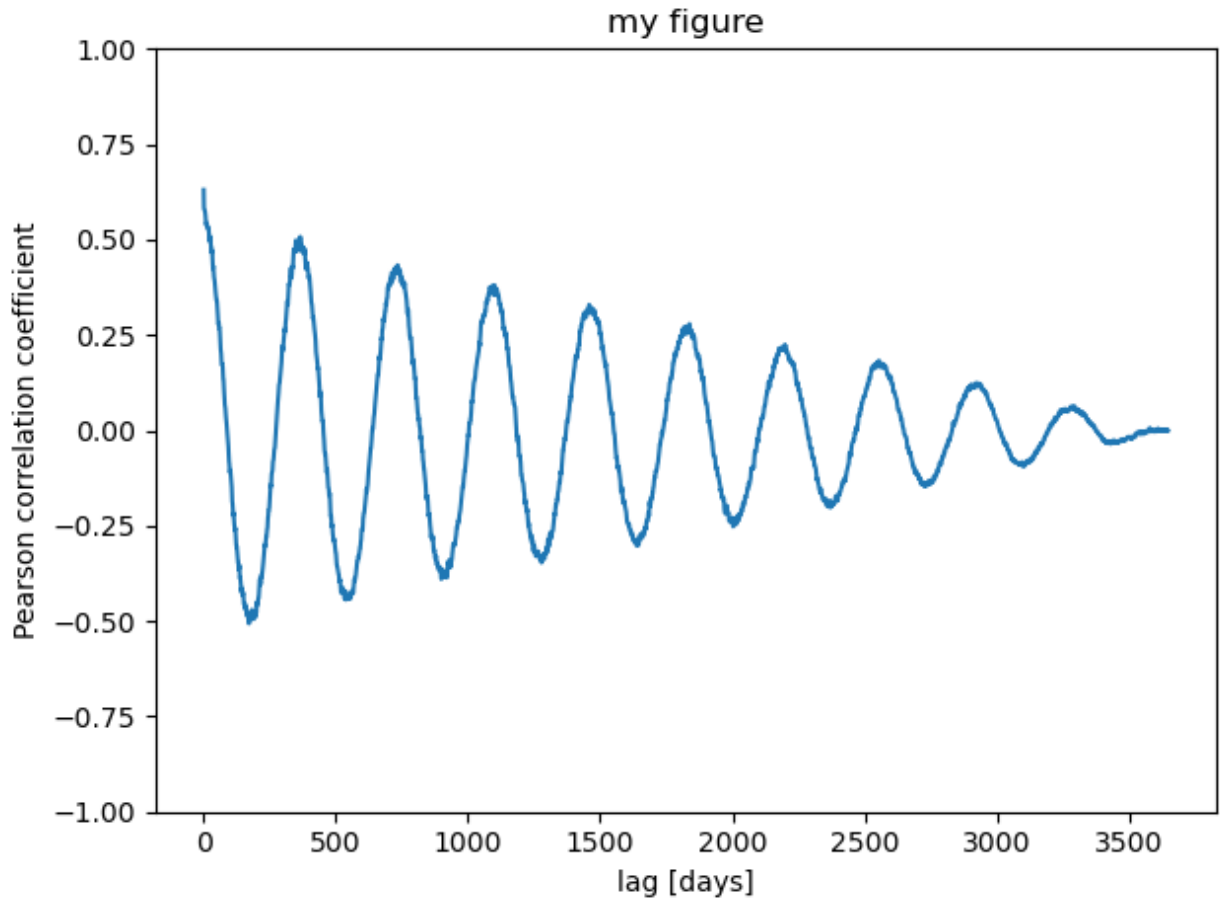
for i in np.arange(len(lags)):
    x = df['Temp'].iloc[i:-1].reset_index(drop=True) # recent observations
    y = df['Temp'].iloc[:i-1].reset_index(drop=True) # lag-shifted observation
    # the shapes must be the same
    if x.shape != y.shape:
        raise ValueError('shape mismatch!')
    # Pearson 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])

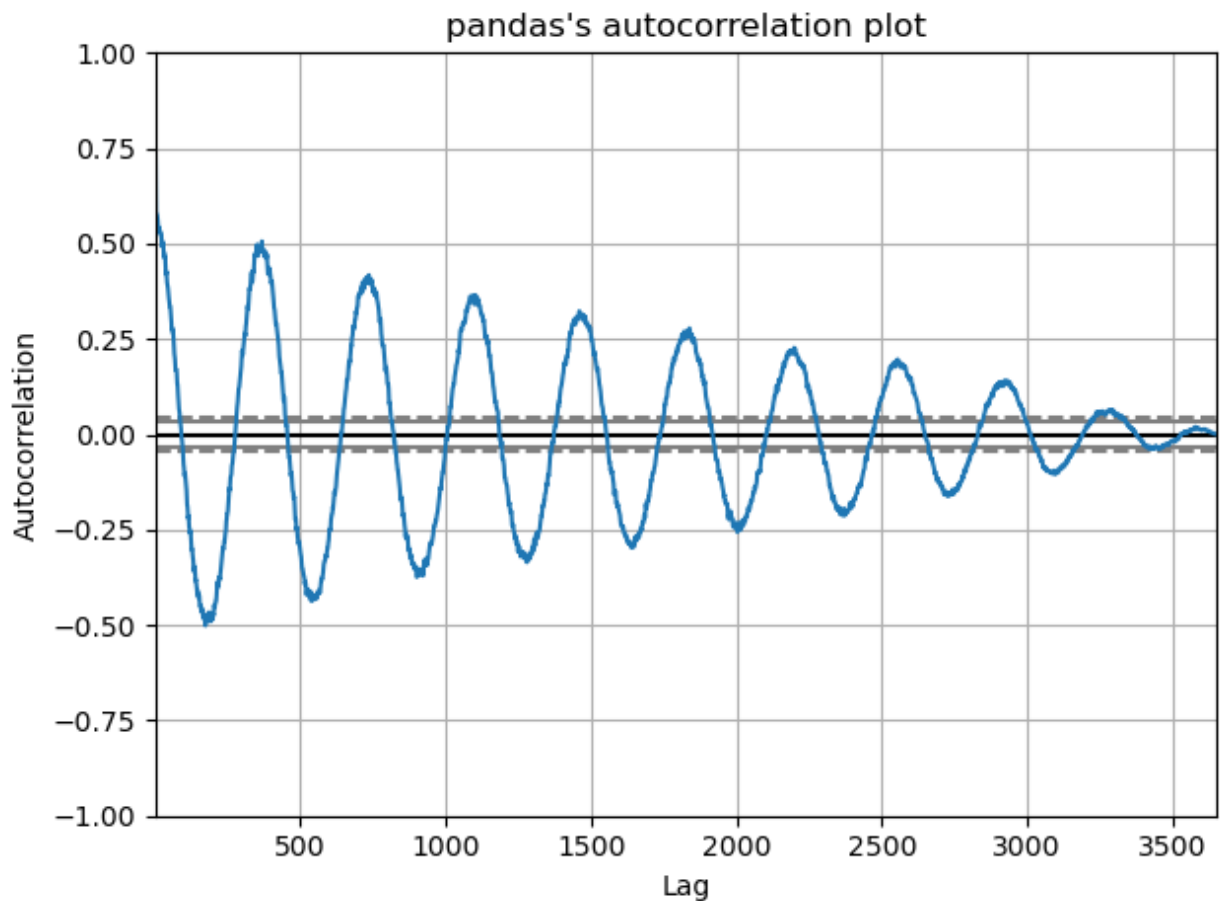
plt.plot(lags[2:], corr_coefs[2:])
plt.ylim([-1, 1])
plt.xlabel('lag [days]')
plt.ylabel('Pearson correlation coefficient')
plt.title('my figure')
plt.tight_layout()
plt.show()

# a one-liner
pd.plotting.autocorrelation_plot(df['Temp'])
plt.title("pandas's autocorrelation plot")
plt.tight_layout()
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/python3.10/site-packages/numpy/li  
b/function_base.py:2821: RuntimeWarning: Degrees of freedom <= 0 for slice  
  c = cov(x, y, rowvar, dtype=dtype)  
/Users/azsom/opt/anaconda3/envs/data1030/lib/python3.10/site-packages/numpy/li  
b/function_base.py:2680: RuntimeWarning: divide by zero encountered in true_di  
vide  
  c *= np.true_divide(1, fact)
```





Autoregression: create 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
... 	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 should still be split based on time (e.g., older observations in train, most recent observations in test)

```
In [12]: y = df['Temp']
X = pd.concat([df['Temp'].shift(3), df['Temp'].shift(2), df['Temp'].shift(1)], axis=1)
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 constant 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 []: