Mudcard

- **When would one want to use a sparse matrix (i.e. the result of setting sparse_output=True for OneHotEncoder) versus the dense array seen in class?**
  - I use the non-sparse output so I can print out the preprocessed matrices in a format that's familiar to everyone.
  - Feel free to try and use sparse matrices though. Here is the description on how they work.
- **Are there ways to write code to check and ensure that each column in the dataset is standard without manually inspecting all the features?**
  - What do you mean by "each column in the dataset is standard"? What does tandard refer to here? Please come to the office hours or post on the course forum.
- **"For fitting and transforming the test vs. train dataset, I am confused in simple terms the process of this. Is it fit only train dataset, and then transform both test and train?**
  - Yes, you fit on the training set and transform all sets.
- **When we use ordinal encoding, do the numbers matter or just that they are in order? For example, after ordinal encoding does a value of 4 mean that this item is twice the weight of a value of 2?**
  - Usually the actual value doesn't matter much, only tht they are in order
  - However, if you know what value should be assigned to each ordinal category, write your own function to perform the transformation.
- **When using time-series data will using a small lag create overfitting?**
  - It might but cross-validation will take care of that. More on this in a few weeks.

Missing values, feature selection and feature engineering

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

- evaluate simple approaches for handling missing values
- engineer features
- select features in supervised ML

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- select features in supervised ML

Dataset

- kaggle house price dataset
- check out the train.csv and the dataset description in the `data` folder!

In [1]:
```python
# read the data
import pandas as pd
import numpy  as np
from sklearn.model_selection import train_test_split

# Let's load the data
df = pd.read_csv('data/train.csv')
# drop the ID
df.drop(columns=['Id'],inplace=True)

# the target variable
y = df['SalePrice']
df.drop(columns=['SalePrice'],inplace=True)
# the unprocessed feature matrix
X = df
print(X.shape)
# the feature names
ftrs = df.columns
print(df.head())
```

```
(1460, 79)
   MSSubClass MSZoning  LotFrontage  LotArea Street Alley LotShape  \
0          60       RL         65.0     8450   Pave   NaN      Reg
1          20       RL         80.0     9600   Pave   NaN      Reg
2          60       RL         68.0    11250   Pave   NaN      IR1
3          70       RL         60.0     9550   Pave   NaN      IR1
4          60       RL         84.0    14260   Pave   NaN      IR1

  LandContour Utilities LotConfig  ... ScreenPorch PoolArea PoolQC Fence  \
0         Lvl    AllPub    Inside  ...           0        0    NaN   NaN
1         Lvl    AllPub       FR2  ...           0        0    NaN   NaN
2         Lvl    AllPub    Inside  ...           0        0    NaN   NaN
3         Lvl    AllPub    Corner  ...           0        0    NaN   NaN
4         Lvl    AllPub       FR2  ...           0        0    NaN   NaN

  MiscFeature MiscVal  MoSold  YrSold  SaleType  SaleCondition
0         NaN       0       2    2008        WD         Normal
1         NaN       0       5    2007        WD         Normal
2         NaN       0       9    2008        WD         Normal
3         NaN       0       2    2006        WD        Abnorml
4         NaN       0      12    2008        WD         Normal

[5 rows x 79 columns]
```

In [2]:
```python
print('data dimensions:',df.shape)
perc_missing_per_ftr = df.isnull().sum(axis=0)/df.shape[0]
print('fraction of missing values in features:')
print(perc_missing_per_ftr[perc_missing_per_ftr > 0])
print('data types of the features with missing values:')
print(df[perc_missing_per_ftr[perc_missing_per_ftr > 0].index].dtypes)
frac_missing = sum(df.isnull().sum(axis=1)!=0)/df.shape[0]
print('fraction of points with missing values:',frac_missing)
```

```
data dimensions: (1460, 79)
fraction of missing values in features:
LotFrontage     0.177397
Alley           0.937671
MasVnrType      0.597260
MasVnrArea      0.005479
BsmtQual        0.025342
BsmtCond        0.025342
BsmtExposure    0.026027
BsmtFinType1    0.025342
BsmtFinType2    0.026027
Electrical      0.000685
FireplaceQu     0.472603
GarageType      0.055479
GarageYrBlt     0.055479
GarageFinish    0.055479
GarageQual      0.055479
GarageCond      0.055479
PoolQC          0.995205
Fence           0.807534
MiscFeature     0.963014
dtype: float64
data types of the features with missing values:
LotFrontage     float64
Alley            object
MasVnrType       object
MasVnrArea      float64
BsmtQual         object
BsmtCond         object
BsmtExposure     object
BsmtFinType1     object
BsmtFinType2     object
Electrical       object
FireplaceQu      object
GarageType       object
GarageYrBlt     float64
GarageFinish     object
GarageQual       object
GarageCond       object
PoolQC           object
Fence            object
MiscFeature      object
dtype: object
fraction of points with missing values: 1.0
```

Simple approaches for handling missing values

- exclude points or features with missing values
- categorical feature: treat missing values as another category
- continuous feature: sklearn's SimpleImputer

Exclude points or features with missing values

- easy to do with pandas
- if missing values were encountered during data collection, it is likely missing values will occur during deployment too
    - what will you do during deployment?
    - by dropping columns/rows, you basically ignore the missing values
    - is it OK to not predict for a datapoint with missing values when the model is deployed?
        - in finance and medical problems, this is not a luxury you will have
- it's OK to temporarily drop a small fraction of rows/columns to quickly train a model and see if the project is feasible
- but if the project makes it to deployment, you will not be able to ignore the issue

Drop points or features with missing values

- not OK for the house price dataset because all points contain some NaNs.

In [3]:
```
print(df.shape)
# by default, rows/points are dropped
df_r = df.dropna()
print(df_r.shape)
# drop features with missing values
df_c = df.dropna(axis=1)
print(df_c.shape)
```
```
(1460, 79)
(0, 79)
(1460, 60)
```

Categorical feature: treat missing values as another category

- the BEST thing you can do!
- already covered in the preprocessing lecture (one hot encoding)
- example: missing values in gender
    - if survey only has options for male/female, missing values are likely because those people are outside the gender binary
    - it is a bad idea to impute (try to guess male or female and thus boxing them into the binary)
- example: native country in the adult data
    - missing data are represented as ` ?`
    - a one-hot encoded feature was assigned to the missing category

In [4]:
```
# read the data
import pandas as pd
import numpy  as np
from sklearn.model_selection import train_test_split

# Let's load the data
df = pd.read_csv('data/train.csv')
# drop the ID
df.drop(columns=['Id'],inplace=True)

# the target variable
y = df['SalePrice']
df.drop(columns=['SalePrice'],inplace=True)
# the unprocessed feature matrix
X = df.values
print(X.shape)
# the feature names
ftrs = df.columns
```
```
(1460, 79)
```

In [5]:
```
random_state = 42

# let's split to train, CV, and test
X_train, X_other, y_train, y_other = train_test_split(df, y, train_size=0.6, random_state=random_state)
X_CV, X_test, y_CV, y_test = train_test_split(X_other, y_other, test_size=0.5, random_state=random_state)

print(X_train.shape)
print(X_CV.shape)
print(X_test.shape)
```
```
(876, 79)
(292, 79)
(292, 79)
```

In [6]:
```
# collect the various features
cat_ftrs = ['MSZoning','Street','Alley','LandContour','LotConfig','Neighborhood','Condition1','Condition2',\
            'BldgType','HouseStyle','RoofStyle','RoofMatl','Exterior1st','Exterior2nd','MasVnrType','Foundation',\
           'Heating','CentralAir','Electrical','GarageType','PavedDrive','MiscFeature','SaleType','SaleCondition']
ordinal_ftrs = ['LotShape','Utilities','LandSlope','ExterQual','ExterCond','BsmtQual','BsmtCond','BsmtExposure',\
               'BsmtFinType1','BsmtFinType2','HeatingQC','KitchenQual','Functional','FireplaceQu','GarageFinish',\
               'GarageQual','GarageCond','PoolQC','Fence']
ordinal_cats = [['Reg','IR1','IR2','IR3'],['AllPub','NoSewr','NoSeWa','ELO'],['Gtl','Mod','Sev'],\
               ['Po','Fa','TA','Gd','Ex'],['Po','Fa','TA','Gd','Ex'],['NA','Po','Fa','TA','Gd','Ex'],\
               ['NA','Po','Fa','TA','Gd','Ex'],['NA','No','Mn','Av','Gd'],['NA','Unf','LwQ','Rec','BLQ','ALQ','GLQ'
```

```
              ['NA','Unf','LwQ','Rec','BLQ','ALQ','GLQ'],['Po','Fa','TA','Gd','Ex'],['Po','Fa','TA','Gd','Ex'],\
              ['Sal','Sev','Maj2','Maj1','Mod','Min2','Min1','Typ'],['NA','Po','Fa','TA','Gd','Ex'],\
              ['NA','Unf','RFn','Fin'],['NA','Po','Fa','TA','Gd','Ex'],['NA','Po','Fa','TA','Gd','Ex'],
              ['NA','Fa','TA','Gd','Ex'],['NA','MnWw','GdWo','MnPrv','GdPrv']]
num_ftrs = ['MSSubClass','LotFrontage','LotArea','OverallQual','OverallCond','YearBuilt','YearRemodAdd',\
            'MasVnrArea','BsmtFinSF1','BsmtFinSF2','BsmtUnfSF','TotalBsmtSF','1stFlrSF','2ndFlrSF',\
            'LowQualFinSF','GrLivArea','BsmtFullBath','BsmtHalfBath','FullBath','HalfBath','BedroomAbvGr',\
            'KitchenAbvGr','TotRmsAbvGrd','Fireplaces','GarageYrBlt','GarageCars','GarageArea','WoodDeckSF',\
            'OpenPorchSF','EnclosedPorch','3SsnPorch','ScreenPorch','PoolArea','MiscVal','MoSold','YrSold']
```

In [7]:

```
# preprocess with pipeline and columntransformer
from sklearn.compose import ColumnTransformer
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import OneHotEncoder
from sklearn.preprocessing import OrdinalEncoder
from sklearn.preprocessing import StandardScaler
from sklearn.impute import SimpleImputer
from sklearn.experimental import enable_iterative_imputer
from sklearn.impute import IterativeImputer
from sklearn.ensemble import RandomForestRegressor

random_state = 42

# one-hot encoder
# We need to replace the NaN with a string first!
categorical_transformer = Pipeline(steps=[
    ('imputer', SimpleImputer(strategy='constant',fill_value='missing')),
    ('onehot', OneHotEncoder(sparse_output=False,handle_unknown='ignore'))])

# ordinal encoder
# We need to replace the NaN with a string first!
ordinal_transformer = Pipeline(steps=[
    ('imputer2', SimpleImputer(strategy='constant',fill_value='NA')),
    ('ordinal', OrdinalEncoder(categories = ordinal_cats))])

# standard scaler
numeric_transformer = Pipeline(steps=[
    ('scaler', StandardScaler())])

# collect the transformers
preprocessor = ColumnTransformer(
    transformers=[
        ('num', numeric_transformer, num_ftrs),
        ('cat', categorical_transformer, cat_ftrs),
        ('ord', ordinal_transformer, ordinal_ftrs)])
```

In [8]:

```
# fit_transform the training set
X_prep = preprocessor.fit_transform(X_train)
# the feature names after fit
feature_names = preprocessor.get_feature_names_out()

# you can convert the numpy array back to a data frame with the feature names if you want
df_train = pd.DataFrame(data=X_prep,columns=feature_names)
print(df_train.shape)

# transform the CV
df_CV = preprocessor.transform(X_CV)
df_CV = pd.DataFrame(data=df_CV,columns = feature_names)
print(df_CV.shape)

# transform the test
df_test = preprocessor.transform(X_test)
df_test = pd.DataFrame(data=df_test,columns = feature_names)
print(df_test.shape)
print(feature_names)
```

```
(876, 222)
(292, 222)
(292, 222)
['num__MSSubClass' 'num__LotFrontage' 'num__LotArea' 'num__OverallQual'
 'num__OverallCond' 'num__YearBuilt' 'num__YearRemodAdd' 'num__MasVnrArea'
 'num__BsmtFinSF1' 'num__BsmtFinSF2' 'num__BsmtUnfSF' 'num__TotalBsmtSF'
 'num__1stFlrSF' 'num__2ndFlrSF' 'num__LowQualFinSF' 'num__GrLivArea'
 'num__BsmtFullBath' 'num__BsmtHalfBath' 'num__FullBath' 'num__HalfBath'
 'num__BedroomAbvGr' 'num__KitchenAbvGr' 'num__TotRmsAbvGrd'
 'num__Fireplaces' 'num__GarageYrBlt' 'num__GarageCars' 'num__GarageArea'
 'num__WoodDeckSF' 'num__OpenPorchSF' 'num__EnclosedPorch'
 'num__3SsnPorch' 'num__ScreenPorch' 'num__PoolArea' 'num__MiscVal'
 'num__MoSold' 'num__YrSold' 'cat__MSZoning_C (all)' 'cat__MSZoning_FV'
 'cat__MSZoning_RH' 'cat__MSZoning_RL' 'cat__MSZoning_RM'
 'cat__Street_Grvl' 'cat__Street_Pave' 'cat__Alley_Grvl' 'cat__Alley_Pave'
 'cat__Alley_missing' 'cat__LandContour_Bnk' 'cat__LandContour_HLS'
 'cat__LandContour_Low' 'cat__LandContour_Lvl' 'cat__LotConfig_Corner'
 'cat__LotConfig_CulDSac' 'cat__LotConfig_FR2' 'cat__LotConfig_FR3'
 'cat__LotConfig_Inside' 'cat__Neighborhood_Blmngtn'
 'cat__Neighborhood_Blueste' 'cat__Neighborhood_BrDale'
 'cat__Neighborhood_BrkSide' 'cat__Neighborhood_ClearCr'
 'cat__Neighborhood_CollgCr' 'cat__Neighborhood_Crawfor'
 'cat__Neighborhood_Edwards' 'cat__Neighborhood_Gilbert'
 'cat__Neighborhood_IDOTRR' 'cat__Neighborhood_MeadowV'
 'cat__Neighborhood_Mitchel' 'cat__Neighborhood_NAmes'
 'cat__Neighborhood_NPkVill' 'cat__Neighborhood_NWAmes'
 'cat__Neighborhood_NoRidge' 'cat__Neighborhood_NridgHt'
 'cat__Neighborhood_OldTown' 'cat__Neighborhood_SWISU'
 'cat__Neighborhood_Sawyer' 'cat__Neighborhood_SawyerW'
 'cat__Neighborhood_Somerst' 'cat__Neighborhood_StoneBr'
 'cat__Neighborhood_Timber' 'cat__Neighborhood_Veenker'
 'cat__Condition1_Artery' 'cat__Condition1_Feedr' 'cat__Condition1_Norm'
 'cat__Condition1_PosA' 'cat__Condition1_PosN' 'cat__Condition1_RRAe'
 'cat__Condition1_RRAn' 'cat__Condition1_RRNe' 'cat__Condition1_RRNn'
 'cat__Condition2_Artery' 'cat__Condition2_Feedr' 'cat__Condition2_Norm'
 'cat__Condition2_PosN' 'cat__Condition2_RRAe' 'cat__Condition2_RRAn'
 'cat__BldgType_1Fam' 'cat__BldgType_2fmCon' 'cat__BldgType_Duplex'
 'cat__BldgType_Twnhs' 'cat__BldgType_TwnhsE' 'cat__HouseStyle_1.5Fin'
 'cat__HouseStyle_1.5Unf' 'cat__HouseStyle_1Story'
 'cat__HouseStyle_2.5Fin' 'cat__HouseStyle_2.5Unf'
 'cat__HouseStyle_2Story' 'cat__HouseStyle_SFoyer' 'cat__HouseStyle_SLvl'
 'cat__RoofStyle_Flat' 'cat__RoofStyle_Gable' 'cat__RoofStyle_Gambrel'
 'cat__RoofStyle_Hip' 'cat__RoofStyle_Mansard' 'cat__RoofStyle_Shed'
 'cat__RoofMatl_ClyTile' 'cat__RoofMatl_CompShg' 'cat__RoofMatl_Metal'
 'cat__RoofMatl_Roll' 'cat__RoofMatl_Tar&Grv' 'cat__RoofMatl_WdShake'
 'cat__RoofMatl_WdShngl' 'cat__Exterior1st_AsbShng'
 'cat__Exterior1st_AsphShn' 'cat__Exterior1st_BrkComm'
 'cat__Exterior1st_BrkFace' 'cat__Exterior1st_CBlock'
 'cat__Exterior1st_CemntBd' 'cat__Exterior1st_HdBoard'
 'cat__Exterior1st_MetalSd' 'cat__Exterior1st_Plywood'
 'cat__Exterior1st_Stone' 'cat__Exterior1st_Stucco'
 'cat__Exterior1st_VinylSd' 'cat__Exterior1st_Wd Sdng'
 'cat__Exterior1st_WdShing' 'cat__Exterior2nd_AsbShng'
 'cat__Exterior2nd_AsphShn' 'cat__Exterior2nd_Brk Cmn'
 'cat__Exterior2nd_BrkFace' 'cat__Exterior2nd_CBlock'
 'cat__Exterior2nd_CmentBd' 'cat__Exterior2nd_HdBoard'
 'cat__Exterior2nd_ImStucc' 'cat__Exterior2nd_MetalSd'
 'cat__Exterior2nd_Other' 'cat__Exterior2nd_Plywood'
 'cat__Exterior2nd_Stone' 'cat__Exterior2nd_Stucco'
 'cat__Exterior2nd_VinylSd' 'cat__Exterior2nd_Wd Sdng'
 'cat__Exterior2nd_Wd Shng' 'cat__MasVnrType_BrkCmn'
 'cat__MasVnrType_BrkFace' 'cat__MasVnrType_Stone'
 'cat__MasVnrType_missing' 'cat__Foundation_BrkTil'
 'cat__Foundation_CBlock' 'cat__Foundation_PConc' 'cat__Foundation_Slab'
 'cat__Foundation_Stone' 'cat__Foundation_Wood' 'cat__Heating_Floor'
 'cat__Heating_GasA' 'cat__Heating_GasW' 'cat__Heating_Grav'
 'cat__Heating_OthW' 'cat__Heating_Wall' 'cat__CentralAir_N'
 'cat__CentralAir_Y' 'cat__Electrical_FuseA' 'cat__Electrical_FuseF'
 'cat__Electrical_FuseP' 'cat__Electrical_SBrkr' 'cat__Electrical_missing'
 'cat__GarageType_2Types' 'cat__GarageType_Attchd'
 'cat__GarageType_Basment' 'cat__GarageType_BuiltIn'
 'cat__GarageType_CarPort' 'cat__GarageType_Detchd'
 'cat__GarageType_missing' 'cat__PavedDrive_N' 'cat__PavedDrive_P'
 'cat__PavedDrive_Y' 'cat__MiscFeature_Gar2' 'cat__MiscFeature_Shed'
 'cat__MiscFeature_TenC' 'cat__MiscFeature_missing' 'cat__SaleType_COD'
 'cat__SaleType_CWD' 'cat__SaleType_Con' 'cat__SaleType_ConLD'
 'cat__SaleType_ConLI' 'cat__SaleType_ConLw' 'cat__SaleType_New'
 'cat__SaleType_Oth' 'cat__SaleType_WD' 'cat__SaleCondition_Abnorml'
 'cat__SaleCondition_AdjLand' 'cat__SaleCondition_Alloca'
 'cat__SaleCondition_Family' 'cat__SaleCondition_Normal'
 'cat__SaleCondition_Partial' 'ord__LotShape' 'ord__Utilities'
 'ord__LandSlope' 'ord__ExterQual' 'ord__ExterCond' 'ord__BsmtQual'
 'ord__BsmtCond' 'ord__BsmtExposure' 'ord__BsmtFinType1'
 'ord__BsmtFinType2' 'ord__HeatingQC' 'ord__KitchenQual' 'ord__Functional'
 'ord__FireplaceQu' 'ord__GarageFinish' 'ord__GarageQual'
 'ord__GarageCond' 'ord__PoolQC' 'ord__Fence']
```

In [9]:
```
print('data dimensions:',df_train.shape)
perc_missing_per_ftr = df_train.isnull().sum(axis=0)/df_train.shape[0]
print('fraction of missing values in features:')
print(perc_missing_per_ftr[perc_missing_per_ftr > 0])
print('data types of the features with missing values:')
print(df_train[perc_missing_per_ftr[perc_missing_per_ftr > 0].index].dtypes)
frac_missing = sum(df_train.isnull().sum(axis=1)!=0)/df_train.shape[0]
print('fraction of points with missing values:',frac_missing)
```

```
data dimensions: (876, 222)
fraction of missing values in features:
num__LotFrontage    0.190639
num__MasVnrArea     0.002283
num__GarageYrBlt    0.052511
dtype: float64
data types of the features with missing values:
num__LotFrontage    float64
num__MasVnrArea     float64
num__GarageYrBlt    float64
dtype: object
fraction of points with missing values: 0.23972602739726026
```

Quiz 1

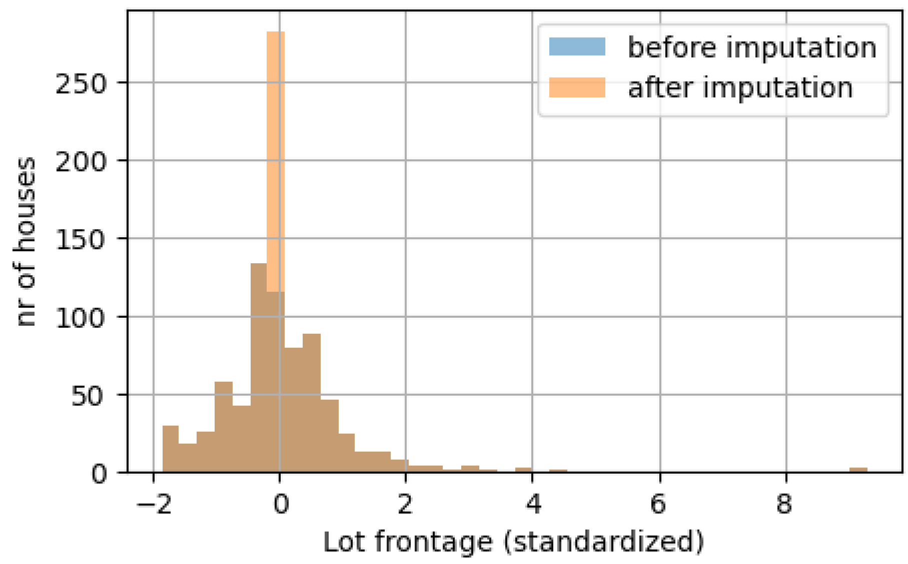
The gender feature below contains missing values. Please explain how you would encode it and would be the output of the encoder. Do not write code. The goal of this quiz is to test your conceptual understanding so write text and the output array.

gender = ['Male', 'Female', 'Male', NaN, NaN, 'Female']

Continuous feature: sklearn's SimpleImputer

- Imputation means you infer the missing values from the known part of the data
- sklearn's SimpleImputer can do mean and median imputation
- A BAD IDEA!
  - mean or median imputation decreases the variance of the feature

In [10]:
```
import matplotlib.pyplot as plt

si = SimpleImputer(strategy='mean')
X_lot = si.fit_transform(df_train[['num__LotFrontage']])

plt.figure(figsize=(5,3))
df_train['num__LotFrontage'].hist(bins=40,label = 'before imputation',alpha=0.5)
plt.hist(X_lot,bins=40,label='after imputation',alpha=0.5)
plt.xlabel('Lot frontage (standardized)')
plt.ylabel('nr of houses')
plt.legend()
plt.show()

print('std before imputation:',np.std(df_train['num__LotFrontage']))
print('std after imputation:',np.std(X_lot))
```




```
std before imputation: 1.0
std after imputation: 0.8996447802291788
```

If your project dataset has missing values...

- handle missing values in categorical and ordinal features as we discussed above
- describe missing values in continuous features
  - how many continuous features contain missing values?
  - what fraction of points contain missing values?
  - what the fraction of missing values in each continuous feature?
- we will cover three advanced methods to handle missing values in continuous features in a few weeks

- multivariate imputation
- XGBoost
- reduced features method (aka the pattern submodel approach)

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

- evaluate simple approaches for handling missing values
- **engineer features**
- select features in supervised ML

Feature engineering

Automatic feature engineering:

- combine features in a simple and automatic way (PolynomialFeatures method in sklearn)
- if n_ftrs << n_points, this can modestly improve the predictive power of your model

Manual feature engineering:

- difficult, project-specific, and requires domain-knowledge
- it can boost the predictive power of your model!

Automatic feature engineering

In [11]:
```
import numpy as np
from sklearn.preprocessing import PolynomialFeatures


X = np.arange(6).reshape(3, 2)
print(X)

poly = PolynomialFeatures(2)
print(poly.fit_transform(X)) # [1, a, b, a^2, ab, b^2]
poly = PolynomialFeatures(2, include_bias=False)
print(poly.fit_transform(X)) # [a, b, a^2, ab, b^2]
poly = PolynomialFeatures(2,interaction_only=True, include_bias=False)
print(poly.fit_transform(X)) # [a, b, ab]
```

```
[[0 1]
 [2 3]
 [4 5]]
[[ 1.  0.  1.  0.  0.  1.]
 [ 1.  2.  3.  4.  6.  9.]
 [ 1.  4.  5. 16. 20. 25.]]
[[ 0.  1.  0.  0.  1.]
 [ 2.  3.  4.  6.  9.]
 [ 4.  5. 16. 20. 25.]]
[[ 0.  1.  0.]
 [ 2.  3.  6.]
 [ 4.  5. 20.]]
```

In [12]:
```
help(PolynomialFeatures)
```

```
Help on class PolynomialFeatures in module sklearn.preprocessing._polynomial:

class PolynomialFeatures(sklearn.base.TransformerMixin, sklearn.base.BaseEstimator)
 |  PolynomialFeatures(degree=2, *, interaction_only=False, include_bias=True, order='C')
 |
 |  Generate polynomial and interaction features.
 |
 |  Generate a new feature matrix consisting of all polynomial combinations
 |  of the features with degree less than or equal to the specified degree.
 |  For example, if an input sample is two dimensional and of the form
 |  [a, b], the degree-2 polynomial features are [1, a, b, a^2, ab, b^2].
 |
 |  Read more in the :ref:`User Guide <polynomial_features>`.
 |
 |  Parameters
 |  ----------
 |  degree : int or tuple (min_degree, max_degree), default=2
 |      If a single int is given, it specifies the maximal degree of the
 |      polynomial features. If a tuple `(min_degree, max_degree)` is passed,
 |      then `min_degree` is the minimum and `max_degree` is the maximum
 |      polynomial degree of the generated features. Note that `min_degree=0`
 |      and `min_degree=1` are equivalent as outputting the degree zero term is
 |      determined by `include_bias`.
 |
 |  interaction_only : bool, default=False
 |      If `True`, only interaction features are produced: features that are
 |      products of at most `degree` *distinct* input features, i.e. terms with
 |      power of 2 or higher of the same input feature are excluded:
 |
 |          - included: `x[0]`, `x[1]`, `x[0] * x[1]`, etc.
 |          - excluded: `x[0] ** 2`, `x[0] ** 2 * x[1]`, etc.
 |
 |  include_bias : bool, default=True
 |      If `True` (default), then include a bias column, the feature in which
 |      all polynomial powers are zero (i.e. a column of ones - acts as an
 |      intercept term in a linear model).
 |
 |  order : {'C', 'F'}, default='C'
 |      Order of output array in the dense case. `'F'` order is faster to
 |      compute, but may slow down subsequent estimators.
 |
 |      .. versionadded:: 0.21
 |
 |  Attributes
 |  ----------
 |  powers_ : ndarray of shape (`n_output_features_`, `n_features_in_`)
 |      `powers_[i, j]` is the exponent of the jth input in the ith output.
 |
 |  n_features_in_ : int
 |      Number of features seen during :term:`fit`.
 |
 |      .. versionadded:: 0.24
 |
 |  feature_names_in_ : ndarray of shape (`n_features_in_`,)
 |      Names of features seen during :term:`fit`. Defined only when `X`
 |      has feature names that are all strings.
 |
 |      .. versionadded:: 1.0
 |
 |  n_output_features_ : int
 |      The total number of polynomial output features. The number of output
 |      features is computed by iterating over all suitably sized combinations
 |      of input features.
 |
 |  See Also
 |  --------
 |  SplineTransformer : Transformer that generates univariate B-spline bases
 |      for features.
 |
 |  Notes
 |  -----
 |  Be aware that the number of features in the output array scales
 |  polynomially in the number of features of the input array, and
 |  exponentially in the degree. High degrees can cause overfitting.
 |
 |  See :ref:`examples/linear_model/plot_polynomial_interpolation.py
 |  <sphx_glr_auto_examples_linear_model_plot_polynomial_interpolation.py>`
 |
 |  Examples
 |  --------
 |  >>> import numpy as np
 |  >>> from sklearn.preprocessing import PolynomialFeatures
 |  >>> X = np.arange(6).reshape(3, 2)
 |  >>> X
 |  array([[0, 1],
 |         [2, 3],
 |         [4, 5]])
```

```
 |  >>> poly = PolynomialFeatures(2)
 |  >>> poly.fit_transform(X)
 |  array([[ 1.,  0.,  1.,  0.,  0.,  1.],
 |         [ 1.,  2.,  3.,  4.,  6.,  9.],
 |         [ 1.,  4.,  5., 16., 20., 25.]])
 |  >>> poly = PolynomialFeatures(interaction_only=True)
 |  >>> poly.fit_transform(X)
 |  array([[ 1.,  0.,  1.,  0.],
 |         [ 1.,  2.,  3.,  6.],
 |         [ 1.,  4.,  5., 20.]])
 |
 |  Method resolution order:
 |      PolynomialFeatures
 |      sklearn.base.TransformerMixin
 |      sklearn.utils._set_output._SetOutputMixin
 |      sklearn.base.BaseEstimator
 |      sklearn.utils._estimator_html_repr._HTMLDocumentationLinkMixin
 |      sklearn.utils._metadata_requests._MetadataRequester
 |      builtins.object
 |
 |  Methods defined here:
 |
 |  __init__(self, degree=2, *, interaction_only=False, include_bias=True, order='C')
 |      Initialize self.  See help(type(self)) for accurate signature.
 |
 |  fit(self, X, y=None)
 |      Compute number of output features.
 |
 |      Parameters
 |      ----------
 |      X : {array-like, sparse matrix} of shape (n_samples, n_features)
 |          The data.
 |
 |      y : Ignored
 |          Not used, present here for API consistency by convention.
 |
 |      Returns
 |      -------
 |      self : object
 |          Fitted transformer.
 |
 |  get_feature_names_out(self, input_features=None)
 |      Get output feature names for transformation.
 |
 |      Parameters
 |      ----------
 |      input_features : array-like of str or None, default=None
 |          Input features.
 |
 |          - If `input_features is None`, then `feature_names_in_` is
 |            used as feature names in. If `feature_names_in_` is not defined,
 |            then the following input feature names are generated:
 |            `["x0", "x1", ..., "x(n_features_in_ - 1)"]`.
 |          - If `input_features` is an array-like, then `input_features` must
 |            match `feature_names_in_` if `feature_names_in_` is defined.
 |
 |      Returns
 |      -------
 |      feature_names_out : ndarray of str objects
 |          Transformed feature names.
 |
 |  transform(self, X)
 |      Transform data to polynomial features.
 |
 |      Parameters
 |      ----------
 |      X : {array-like, sparse matrix} of shape (n_samples, n_features)
 |          The data to transform, row by row.
 |
 |          Prefer CSR over CSC for sparse input (for speed), but CSC is
 |          required if the degree is 4 or higher. If the degree is less than
 |          4 and the input format is CSC, it will be converted to CSR, have
 |          its polynomial features generated, then converted back to CSC.
 |
 |          If the degree is 2 or 3, the method described in "Leveraging
 |          Sparsity to Speed Up Polynomial Feature Expansions of CSR Matrices
 |          Using K-Simplex Numbers" by Andrew Nystrom and John Hughes is
 |          used, which is much faster than the method used on CSC input. For
 |          this reason, a CSC input will be converted to CSR, and the output
 |          will be converted back to CSC prior to being returned, hence the
 |          preference of CSR.
 |
 |      Returns
 |      -------
 |      XP : {ndarray, sparse matrix} of shape (n_samples, NP)
 |          The matrix of features, where `NP` is the number of polynomial
 |          features generated from the combination of inputs. If a sparse
```

```
 |          matrix is provided, it will be converted into a sparse
 |          `csr_matrix`.
 |  
 |  ----------------------------------------------------------------------
 |  Readonly properties defined here:
 |  
 |  powers_
 |      Exponent for each of the inputs in the output.
 |  
 |  ----------------------------------------------------------------------
 |  Data and other attributes defined here:
 |  
 |  __annotations__ = {'_parameter_constraints': <class 'dict'>}
 |  
 |  ----------------------------------------------------------------------
 |  Methods inherited from sklearn.base.TransformerMixin:
 |  
 |  fit_transform(self, X, y=None, **fit_params)
 |      Fit to data, then transform it.
 |      
 |      Fits transformer to `X` and `y` with optional parameters `fit_params`
 |      and returns a transformed version of `X`.
 |      
 |      Parameters
 |      ----------
 |      X : array-like of shape (n_samples, n_features)
 |          Input samples.
 |      
 |      y :  array-like of shape (n_samples,) or (n_samples, n_outputs),                 default=None
 |          Target values (None for unsupervised transformations).
 |      
 |      **fit_params : dict
 |          Additional fit parameters.
 |      
 |      Returns
 |      -------
 |      X_new : ndarray array of shape (n_samples, n_features_new)
 |          Transformed array.
 |  
 |  ----------------------------------------------------------------------
 |  Methods inherited from sklearn.utils._set_output._SetOutputMixin:
 |  
 |  set_output(self, *, transform=None)
 |      Set output container.
 |      
 |      See :ref:`sphx_glr_auto_examples_miscellaneous_plot_set_output.py`
 |      for an example on how to use the API.
 |      
 |      Parameters
 |      ----------
 |      transform : {"default", "pandas", "polars"}, default=None
 |          Configure output of `transform` and `fit_transform`.
 |      
 |          - `"default"`: Default output format of a transformer
 |          - `"pandas"`: DataFrame output
 |          - `"polars"`: Polars output
 |          - `None`: Transform configuration is unchanged
 |      
 |          .. versionadded:: 1.4
 |              `"polars"` option was added.
 |      
 |      Returns
 |      -------
 |      self : estimator instance
 |          Estimator instance.
 |  
 |  ----------------------------------------------------------------------
 |  Class methods inherited from sklearn.utils._set_output._SetOutputMixin:
 |  
 |  __init_subclass__(auto_wrap_output_keys=('transform',), **kwargs)
 |      Set the ``set_{method}_request`` methods.
 |      
 |      This uses PEP-487 [1]_ to set the ``set_{method}_request`` methods. It
 |      looks for the information available in the set default values which are
 |      set using ``__metadata_request__*`` class attributes, or inferred
 |      from method signatures.
 |      
 |      The ``__metadata_request__*`` class attributes are used when a method
 |      does not explicitly accept a metadata through its arguments or if the
 |      developer would like to specify a request value for those metadata
 |      which are different from the default ``None``.
 |      
 |      References
 |      ----------
 |      .. [1] https://www.python.org/dev/peps/pep-0487
 |  
 |  ----------------------------------------------------------------------
```

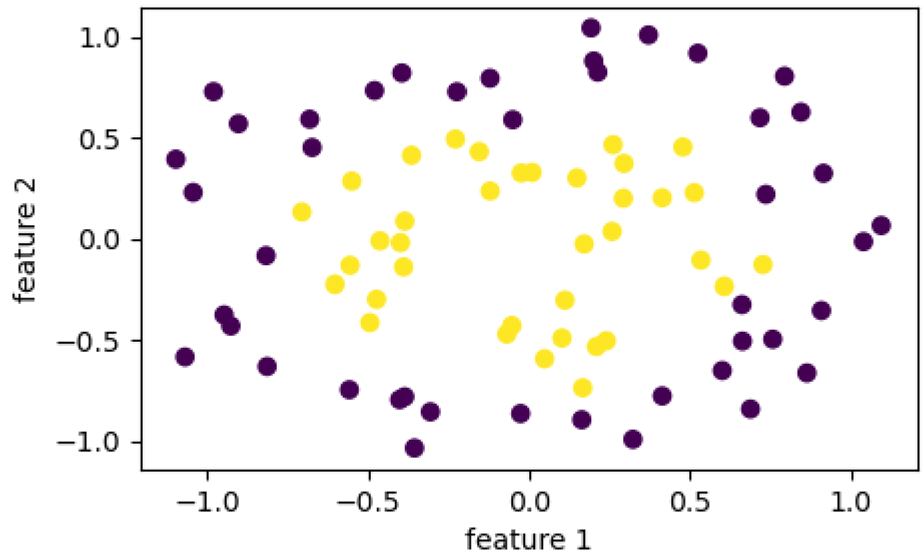
```
 |  Data descriptors inherited from sklearn.utils._set_output._SetOutputMixin:
 |  
 |  __dict__
 |      dictionary for instance variables
 |  
 |  __weakref__
 |      list of weak references to the object
 |  
 |  ----------------------------------------------------------------------
 |  Methods inherited from sklearn.base.BaseEstimator:
 |  
 |  __getstate__(self)
 |      Helper for pickle.
 |  
 |  __repr__(self, N_CHAR_MAX=700)
 |      Return repr(self).
 |  
 |  __setstate__(self, state)
 |  
 |  __sklearn_clone__(self)
 |  
 |  get_params(self, deep=True)
 |      Get parameters for this estimator.
 |      
 |      Parameters
 |      ----------
 |      deep : bool, default=True
 |          If True, will return the parameters for this estimator and
 |          contained subobjects that are estimators.
 |      
 |      Returns
 |      -------
 |      params : dict
 |          Parameter names mapped to their values.
 |  
 |  set_params(self, **params)
 |      Set the parameters of this estimator.
 |      
 |      The method works on simple estimators as well as on nested objects
 |      (such as :class:`~sklearn.pipeline.Pipeline`). The latter have
 |      parameters of the form ``<component>__<parameter>`` so that it's
 |      possible to update each component of a nested object.
 |      
 |      Parameters
 |      ----------
 |      **params : dict
 |          Estimator parameters.
 |      
 |      Returns
 |      -------
 |      self : estimator instance
 |          Estimator instance.
 |  
 |  ----------------------------------------------------------------------
 |  Methods inherited from sklearn.utils._metadata_requests._MetadataRequester:
 |  
 |  get_metadata_routing(self)
 |      Get metadata routing of this object.
 |      
 |      Please check :ref:`User Guide <metadata_routing>` on how the routing
 |      mechanism works.
 |      
 |      Returns
 |      -------
 |      routing : MetadataRequest
 |          A :class:`~sklearn.utils.metadata_routing.MetadataRequest` encapsulating
 |          routing information.
```

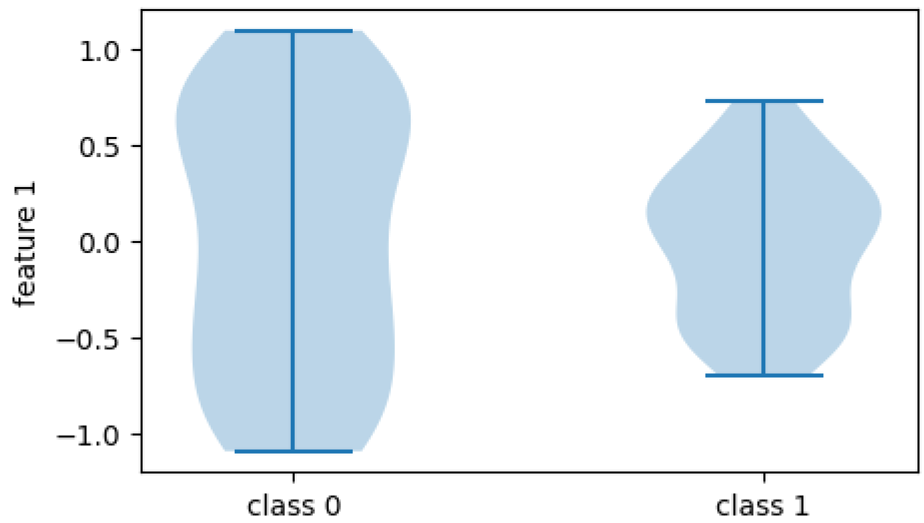
Manual feature engineering

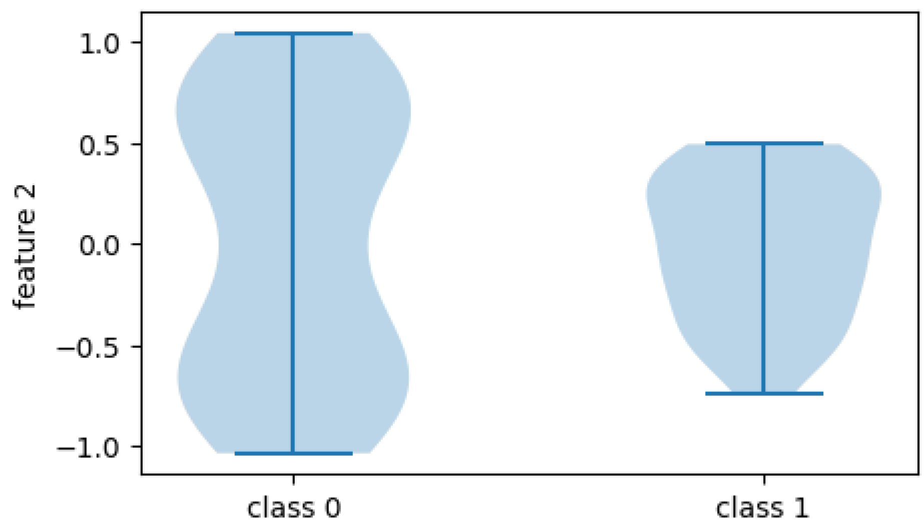
Some advice:

- EDA can give you insights on how you should engineer and preprocess your features better
- normalizing a feature with another feature can often be helpful
  - for example you want to predict who will attend an event
  - two features you have:
    - number of invite emails sent: [10, 20, 10, 20, 5]
    - number of email invites opened: [5, 2, 10, 10, 0]
  - a good new feature could be the fraction of invite emails opened
    - fraction of invite emails opened: [0.5, 0.1, 1, 0.5, 0]
    - person 3 might be more likely to attend than person 2 but that's only obvious from the normalized feature

In [13]:
```
from sklearn.datasets import make_circles
from sklearn.model_selection import train_test_split

X, y = make_circles(noise=0.15, factor=0.5, random_state=1)

X_train, X_test, y_train, y_test = train_test_split(X,y,test_size=0.2,random_state =0)

plt.figure(figsize=(5,3))
plt.scatter(X_train[:,0],X_train[:,1],c=y_train)
plt.xlabel('feature 1')
plt.ylabel('feature 2')
plt.show()

dataset = [X_train[y_train==0,0],
           X_train[y_train==1,0]]

plt.figure(figsize=(5,3))
plt.violinplot(dataset = dataset)
plt.xticks([1,2],['class 0','class 1'])
plt.ylabel('feature 1')
plt.show()


dataset = [X_train[y_train==0,1],
           X_train[y_train==1,1]]

plt.figure(figsize=(5,3))
plt.violinplot(dataset = dataset)
plt.xticks([1,2],['class 0','class 1'])
plt.ylabel('feature 2')
plt.show()
```







In [14]:
```
from sklearn.linear_model import LogisticRegression
from sklearn.metrics import accuracy_score
from matplotlib.colors import ListedColormap
```

```
def simple_ML_pipeline(X_train,X_test,y_train,y_test):
    LR = LogisticRegression() # logistic regression is a simple linear classifier
    LR.fit(X_train,y_train)
    y_test_pred = LR.predict(X_test)
    return accuracy_score(y_test,y_test_pred)

test_score = simple_ML_pipeline(X_train,X_test,y_train,y_test)
print(test_score)
```

```
0.3
```

In [15]:

```
# add new feature
new_feature = np.sqrt(X_train[:,0]**2+X_train[:,1]**2) # the distance from the origin
X_train = np.hstack((X_train,np.expand_dims(new_feature,axis=1)))
print(X_train[:5,:])
new_feature = np.sqrt(X_test[:,0]**2+X_test[:,1]**2)
X_test = np.hstack((X_test,np.expand_dims(new_feature,axis=1)))
```

```
[[-0.05045148  0.58776084  0.58992217]
 [-0.54933449  0.28364692  0.61824264]
 [-0.55471872 -0.13344625  0.57054426]
 [-0.90194371  0.56791184  1.06584535]
 [ 0.41429957 -0.77851327  0.88188834]]
```

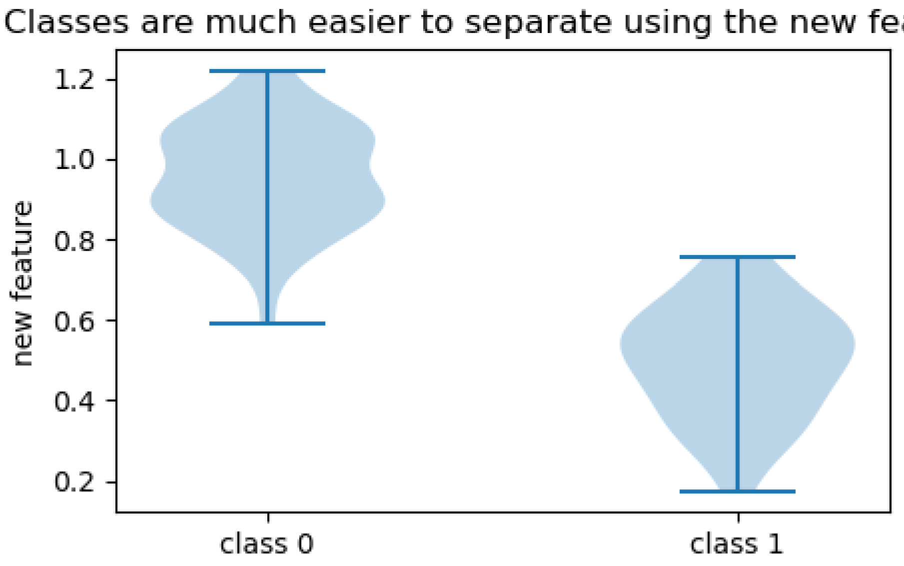
In [16]:

```
test_score = simple_ML_pipeline(X_train,X_test,y_train,y_test)
print(test_score) # the test accuracy improved a lot!
```

```
1.0
```

In [17]:

```
dataset = [X_train[y_train==0,2],
           X_train[y_train==1,2]]

plt.figure(figsize=(5,3))
plt.violinplot(dataset = dataset)
plt.xticks([1,2],['class 0','class 1'])
plt.ylabel('new feature')
plt.title('Classes are much easier to separate using the new feature!')
plt.show()
```



Quiz 2

X has three columns: a, b, and c.

```
X = np.arange(9).reshape(3, 3)

poly = PolynomialFeatures(degree = 2, include_bias = False)
print(poly.fit_transform(X))
```

What will be the shape of the transformed X? Do not run the code. Work the problem out with pen and paper or in your head.

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

- evaluate simple approaches for handling missing values
- engineer features
- **select features in supervised ML**

Feature selection

We cover today how to do feature selection **before** the ML model is trained. We cover later how to select features with ML feature importances.

Necessary if

- you have too many features: n_ftrs > n_points (some algorithms break down)
- if training an ML algorithm is too computationally expensive using all the features

Approach

1. You calculate a single number metric between each feature and the target variable **using the training data only**.

- sklearn supported metrics (for both regression and classification)
  - F test (only measures linear dependency)
  - mutual information (measures non-linear dependency)
- steps:
  - do you work with a classification or regression problem?
    - regression:
      - are you interested in linear or non-linear correlations with the target variable?
        - linear: use `sklearn.feature_selection.f_regression`
        - non-linear: use `sklearn.feature_selection.mutual_info_regression`
    - classification:
      - are you interested in linear or non-linear correlations with the target variable?
        - linear: use `sklearn.feature_selection.f_classif`
        - non-linear: use `sklearn.feature_selection.mutual_info_classif`

2. Keep k best features (`sklearn.feature_selection.SelectKBest` method) or keep a certain percentile of the best features (`sklearn.feature_selection.SelectPercentile` method).

Pros:

- easy to do
- it is quicker to train ML models with fewer features

Cons:

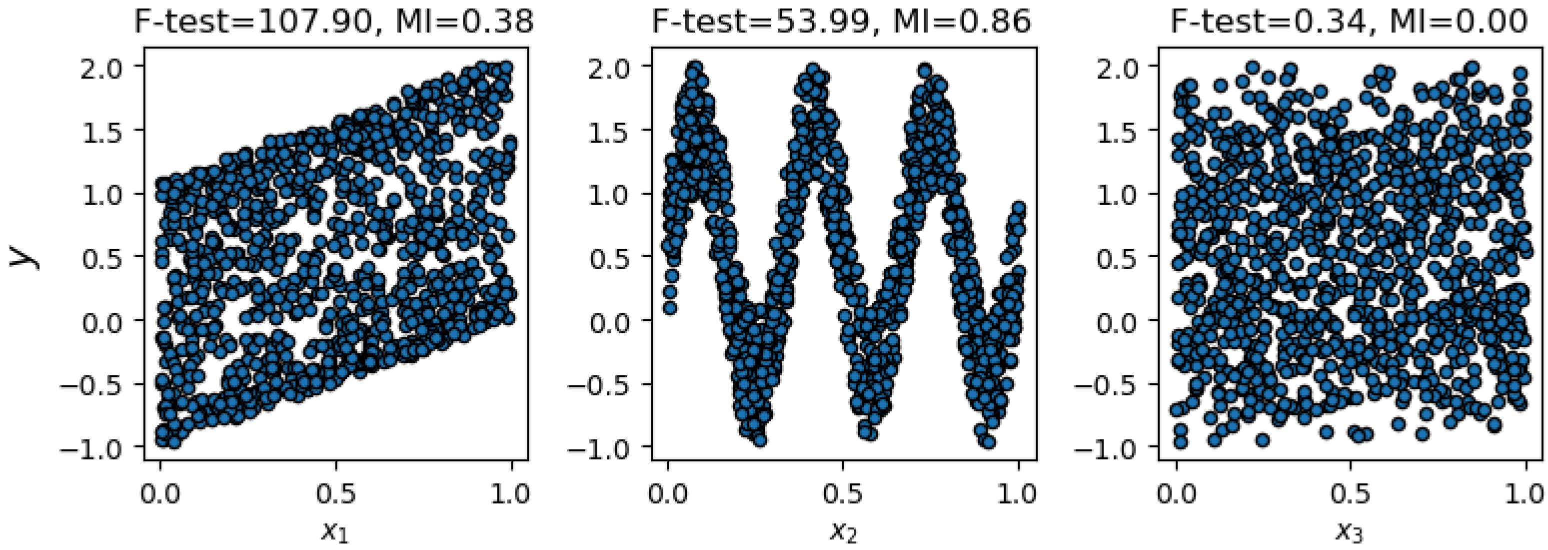
- feature interactions are not taken into account
  - two features separately are not predictive, but they are predictive together - such effects are ignored!

Example

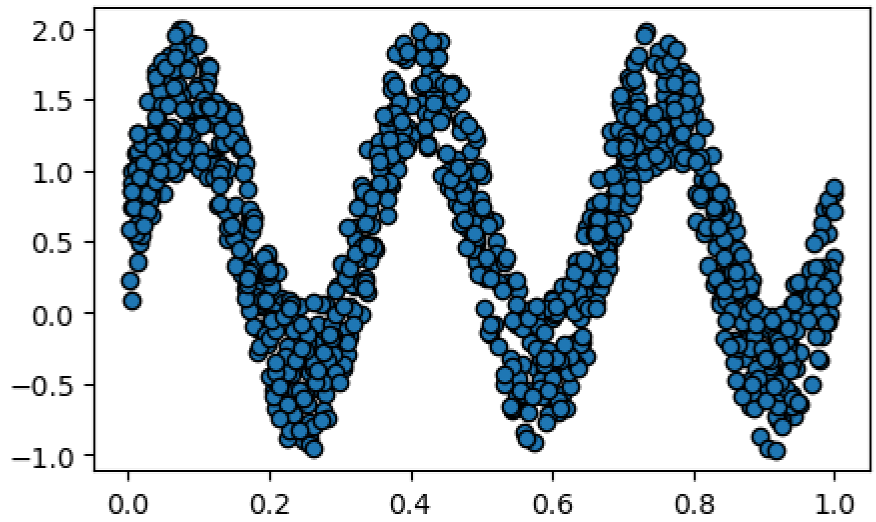
In [18]:
```
import numpy as np
import matplotlib.pyplot as plt
from sklearn.feature_selection import f_regression, mutual_info_regression
np.random.seed(10)

X = np.random.rand(1000,3)
y = X[:,0] + np.sin(6 * np.pi * X[:,1]) + 0.1 * X[:,2]

f_test, p_values = f_regression(X, y)
print('f score',f_test)
print('p values',p_values)
mi = mutual_info_regression(X, y)
print('mi',mi)
```

```
f score [107.90134156  53.99212018   0.34354216]
p values [4.52216746e-24 4.18146945e-13 5.57924253e-01]
mi [0.37637501 0.86317726 0.        ]
```

In [19]:
```
#plt.figure(figsize=(15, 5))
plt.figure(figsize=(8,3))
for i in range(3):
    plt.subplot(1, 3, i + 1)
    plt.scatter(X[:, i], y, edgecolor='black', s=20)
    plt.xlabel("$x_{}$".format(i + 1), fontsize=10)
    if i == 0:
        plt.ylabel("$y$", fontsize=14)
    plt.title("F-test={:.2f}, MI={:.2f}".format(f_test[i], mi[i]),
              fontsize=12)
plt.tight_layout()
plt.show()
```

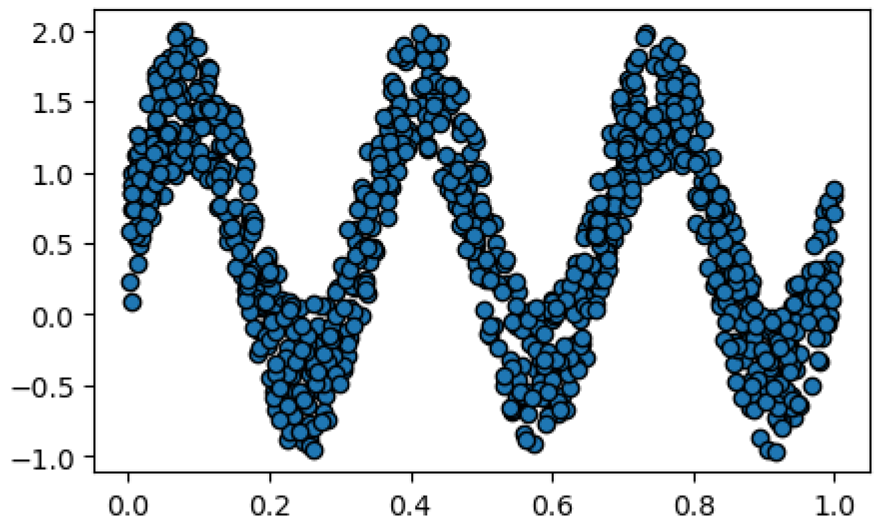


In [20]:
```
from sklearn.feature_selection import SelectKBest
f_select = SelectKBest(mutual_info_regression,k=1)
X_f = f_select.fit_transform(X,y)

plt.figure(figsize=(5,3))
plt.scatter(X_f,y,edgecolor='k')
plt.show()
# the features selected:
print(f_select.get_support())
```



```
[False  True False]
```

In [21]:
```
from sklearn.feature_selection import SelectPercentile
f_selector = SelectPercentile(mutual_info_regression,percentile=33)
X_mi = f_selector.fit_transform(X,y)

plt.figure(figsize=(5,3))
plt.scatter(X_mi,y,edgecolor='k')
plt.show()
# features selected
f_selector.get_support()
```



Out[21]:
```
array([False,  True, False])
```

Be careful though!

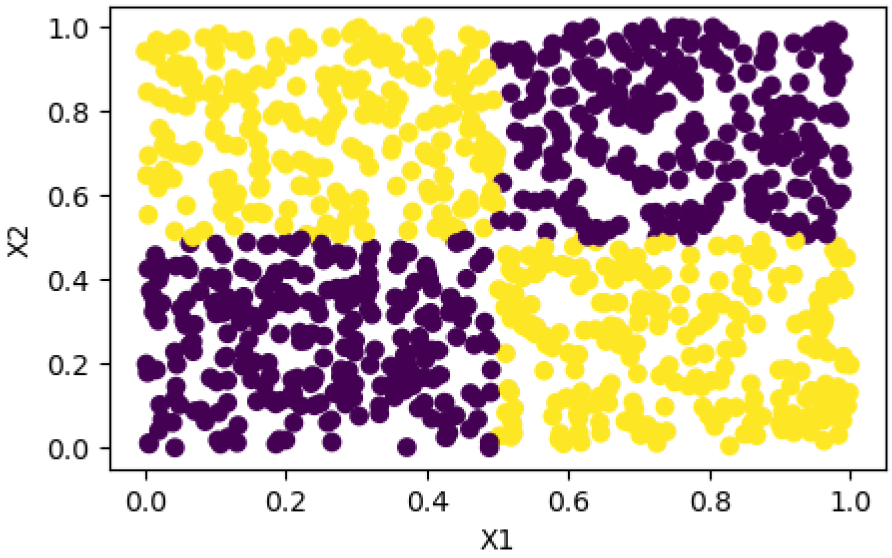
In [22]:
```
# toy data
import pandas as pd
import numpy as np
from sklearn.feature_selection import f_classif, mutual_info_classif
np.random.seed(0)

X = np.random.uniform(size=(1000,2))

y = np.zeros(1000)
```

```
y[(X[:,0]>=0.5)&(X[:,1]<0.5)] = 1
y[(X[:,0]<=0.5)&(X[:,1]>0.5)] = 1
```

In [23]:
```
f_test, p_values = f_classif(X, y)
print('f score',f_test)
print('p values',p_values)

mi = mutual_info_classif(X, y)
print('mi',mi)
```

```
f score [0.28282382 0.82026181]
p values [0.59497468 0.36532223]
mi [0.00338502 0.00055867]
```

In [24]:
```
plt.figure(figsize=(5,3))
plt.scatter(X[:,0],X[:,1],c=y)
plt.xlabel('X1')
plt.ylabel('X2')
plt.show()
```



Mudcard