missing_data_in_supervised_ML

January 15, 2021

##

Missing data in supervised ML

###

Andras Zsom

Lead Data Scientist and Adjunct Lecturer in Data Science

Center for Computation and Visualization

Brown University

0.1 About me

- Born and raised in Hungary
- Astrophysics PhD at MPIA, Heidelberg, Germany
- Postdoctoral researcher at MIT (still in astrophysics at the time)
- Started at Brown in December 2015 as a Data Scientist
- Promoted to Lead Data Scientist in 2017
- Adjunct Lecturer in Data Science last fall and this fall
  - Teaching the course *DATA1030: Hands-on data science*, a mandatory course in the Data Science master's program at Brown

0.2 Data Science at Brown

- Center for Computation and Visualization (CCV) - https://ccv.brown.edu/
- Institutional Data group
  - Data-driven decision support and predictive modeling for Brown's administrative units
  - Academic research on data-intensive projects
  - Data science consulting for industry partners

0.3 Learning Objectives

By the end of this workshop, you will be able to - Describe the three main types of missingness patterns - Evaluate simple approaches for handling missing values - Apply XGBoost to a dataset with missing values - Apply multivariate imputation - Apply the reduced-features model (also called the pattern submodel approach) - Decide which approach is best for your dataset

0.4 Before we start, a few words on our dataset: kaggle house price

- good for educational purposes
  - messy data that requires quite a bit of preprocessing
  - a nice mixture of continuous, ordinal, and categorical features, each feature type has missing values
- lots of excellent kernels on kaggle
  - check them out here
- dataset and description available in repo
  - let's take a look!

0.5 Missing values often occur in datasets

- survey data: not everyone answers all the questions
- medical data: not all tests/treatments/etc are performed on all patients
- sensor can be offline or malfunctioning

0.6 Missing values are an issue for multiple reasons

Conceptual reason

- missing values can introduce biases
  - bias: the samples (the data points) are not representative of the underlying distribution/population
  - any conclusion drawn from a biased dataset is also biased.
  - rich people tend to not fill out survey questions about their salaries and the mean salary estimated from survey data tend to be lower than true value

Practical reason

- missing values (NaN, NA, inf) are incompatible with sklearn
  - all values in an array need to be numerical otherwise sklearn will throw a *ValueError*
- there are a few supervised ML techniques that work with missing values (e.g., XGBoost, CatBoost)
  - we will cover those later today

0.7 Learning Objectives

By the end of this workshop, you will be able to - **Describe the three main types of missingness patterns** - Evaluate simple approaches for handling missing values - Apply XGBoost to a dataset with missing values - Apply multivariate imputation - Apply the reduced-features model (also called the pattern submodel approach) - Decide which approach is best for your dataset

1 Missing data patterns

- **MCAR** - Missing Complete At Random
  - some people skip some survey questions by accident
- **MAR** - Missing At Random
  - males are less likely to fill out a survey on depression
  - this has nothing to do with their level of depression after accounting for maleness

- **MNAR** - Missing Not At Random
  - depressed people are less likely to fill out a survey on depression due to their level of depression

1.1 MCAR test

- MCAR can be diagnosed with a statistical test (Little, 1988)
  - python implementation available in the pymice package or in the skipped slide
- Caveat: it can differentiate between MCAR and MAR only, it misses MNAR

[1]:
```python
# from the pymice package
# https://github.com/RianneSchouten/pymice

import numpy as np
import pandas as pd
import math as ma
import scipy.stats as st

def checks_input_mcar_tests(data):
    """ Checks whether the input parameter of class McarTests is correct
            Parameters
            ----------
            data:
                The input of McarTests specified as 'data'
            Returns
            -------
            bool
                True if input is correct
            """

    if not isinstance(data, pd.DataFrame):
        print("Error: Data should be a Pandas DataFrame")
        return False

    if not any(data.dtypes.values == np.float):
        if not any(data.dtypes.values == np.int):
            print("Error: Dataset cannot contain other value types than floats␣
↪and/or integers")
            return False

    if not data.isnull().values.any():
        print("Error: No NaN's in given data")
        return False

    return True


def mcar_test(data):
```

```
    """ Implementation of Little's MCAR test
    Parameters
    ----------
    data: Pandas DataFrame
        An incomplete dataset with samples as index and variables as columns
    Returns
    -------
    p_value: Float
        This value is the outcome of a chi-square statistical test, testing␣
↪whether the null hypothesis
        'the missingness mechanism of the incomplete dataset is MCAR' can be␣
↪rejected.
    """

    if not checks_input_mcar_tests(data):
        raise Exception("Input not correct")

    dataset = data.copy()
    vars = dataset.dtypes.index.values
    n_var = dataset.shape[1]

    # mean and covariance estimates
    # ideally, this is done with a maximum likelihood estimator
    gmean = dataset.mean()
    gcov = dataset.cov()

    # set up missing data patterns
    r = 1 * dataset.isnull()
    mdp = np.dot(r, list(map(lambda x: ma.pow(2, x), range(n_var))))
    sorted_mdp = sorted(np.unique(mdp))
    n_pat = len(sorted_mdp)
    correct_mdp = list(map(lambda x: sorted_mdp.index(x), mdp))
    dataset['mdp'] = pd.Series(correct_mdp, index=dataset.index)

    # calculate statistic and df
    pj = 0
    d2 = 0
    for i in range(n_pat):
        dataset_temp = dataset.loc[dataset['mdp'] == i, vars]
        select_vars = ~dataset_temp.isnull().any()
        pj += np.sum(select_vars)
        select_vars = vars[select_vars]
        means = dataset_temp[select_vars].mean() - gmean[select_vars]
        select_cov = gcov.loc[select_vars, select_vars]
        mj = len(dataset_temp)
        parta = np.dot(means.T, np.linalg.solve(select_cov, np.
↪identity(select_cov.shape[1])))
```

```
        d2 += mj * (np.dot(parta, means))

    df = pj - n_var

    # perform test and save output
    p_value = 1 - st.chi2.cdf(d2, df)

    return p_value
```

1.2 MCAR, MAR, MNAR are nice in theory, pretty useless in practice

- it can be challenging to infer the missingness pattern from an incomplete dataset
  - There is a statistical test to differentiate MCAR and MAR
  - MNAR is difficult/impossible to diagnose to the best of my knowledge
- multiple patterns can be present in the data
  - even worse, multiple patterns can be present in one feature!
  - missing values in a feature can occur due to a mix of MCAR, MAR, MNAR

1.3 Learning Objectives

By the end of this workshop, you will be able to - Describe the three main types of missingness patterns - **Evaluate simple approaches for handling missing values** - Apply XGBoost to a dataset with missing values - Apply multivariate imputation - Apply the reduced-features model (also called the pattern submodel approach) - Decide which approach is best for your dataset

1.4 Simple approaches for handling missing values

- 1) categorical/ordinal features: treat missing values as another category

  - missing values in categorical/ordinal features are not a big deal

- 2) continuous features: this is the tough part

  - sklearn's SimpleImputer

- 3) exclude points or features with missing values

  - might be OK

1.4.1 1a) Missing values in a categorical feature

- YAY - this is not an issue at all!
- Categorical feature needs to be one-hot encoded anyway
- Just replace the missing values with 'NA' or 'missing' and treat it as a separate category

1.4.2 1b) Missing values in a ordinal feature

- this can be a bit trickier but usually fine
- Ordinal encoder is applied to ordinal features
  - where does 'NA' or 'missing' fit into the order of the categories?
  - usually first or last

- if you can figure this out, you are done

[2]:
```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.values
print(X.shape)
# the feature names
ftrs = df.columns
```

```
(1460, 79)
```

[3]:
```python
# let's split to train, test, and holdout
X_other, X_holdout, y_other, y_holdout = train_test_split(df, y, test_size=0.2,␣
 ↪random_state=0)
X_train, X_test, y_train, y_test = train_test_split(X_other, y_other,␣
 ↪test_size=0.25, random_state=0)

print(X_train.shape)
print(X_test.shape)
print(X_holdout.shape)
```

```
(876, 79)
(292, 79)
(292, 79)
```

[4]:
```python
# collect the various features
cat_ftrs =␣
 ↪['MSZoning','Street','Alley','LandContour','LotConfig','Neighborhood','Condition1','Conditi
          ␣
 ↪'BldgType','HouseStyle','RoofStyle','RoofMatl','Exterior1st','Exterior2nd','MasVnrType','Fo
         ␣
 ↪'Heating','CentralAir','Electrical','GarageType','PavedDrive','MiscFeature','SaleType','Sal
ordinal_ftrs =␣
 ↪['LotShape','Utilities','LandSlope','ExterQual','ExterCond','BsmtQual','BsmtCond','BsmtExpo
```

```
     ␣
↪'BsmtFinType1','BsmtFinType2','HeatingQC','KitchenQual','Functional','FireplaceQu','GarageF
                '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','A
     ␣
↪['NA','Unf','LwQ','Rec','BLQ','ALQ','GLQ'],['Po','Fa','TA','Gd','Ex'],['Po','Fa','TA','Gd',
     ␣
↪['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','BedroomAbvG
    ␣
↪'KitchenAbvGr','TotRmsAbvGrd','Fireplaces','GarageYrBlt','GarageCars','GarageArea','WoodDec
    ␣
↪'OpenPorchSF','EnclosedPorch','3SsnPorch','ScreenPorch','PoolArea','MiscVal','MoSold','YrSo
```

[5]:
```
df[ordinal_ftrs]
```

[5]:
```
     LotShape Utilities LandSlope ExterQual ExterCond BsmtQual BsmtCond  \
0         Reg    AllPub       Gtl        Gd        TA       Gd       TA
1         Reg    AllPub       Gtl        TA        TA       Gd       TA
2         IR1    AllPub       Gtl        Gd        TA       Gd       TA
3         IR1    AllPub       Gtl        TA        TA       TA       Gd
4         IR1    AllPub       Gtl        Gd        TA       Gd       TA
…       …       …       …       …       …       …     …
1455      Reg    AllPub       Gtl        TA        TA       Gd       TA
1456      Reg    AllPub       Gtl        TA        TA       Gd       TA
1457      Reg    AllPub       Gtl        Ex        Gd       TA       Gd
1458      Reg    AllPub       Gtl        TA        TA       TA       TA
1459      Reg    AllPub       Gtl        Gd        TA       TA       TA

     BsmtExposure BsmtFinType1 BsmtFinType2 HeatingQC KitchenQual Functional  \
0              No          GLQ          Unf        Ex          Gd        Typ
1              Gd          ALQ          Unf        Ex          TA        Typ
2              Mn          GLQ          Unf        Ex          Gd        Typ
```

```
3              No          ALQ          Unf         Gd          Gd         Typ
4              Av          GLQ          Unf         Ex          Gd         Typ
…           …          …          …          …         …        …
1455           No          Unf          Unf         Ex          TA         Typ
1456           No          ALQ          Rec         TA          TA        Min1
1457           No          GLQ          Unf         Ex          Gd         Typ
1458           Mn          GLQ          Rec         Gd          Gd         Typ
1459           No          BLQ          LwQ         Gd          TA         Typ

     FireplaceQu GarageFinish GarageQual GarageCond PoolQC  Fence
0            NaN          RFn         TA         TA    NaN    NaN
1             TA          RFn         TA         TA    NaN    NaN
2             TA          RFn         TA         TA    NaN    NaN
3             Gd          Unf         TA         TA    NaN    NaN
4             TA          RFn         TA         TA    NaN    NaN
…          …          …        …        …    …    …
1455          TA          RFn         TA         TA    NaN    NaN
1456          TA          Unf         TA         TA    NaN  MnPrv
1457          Gd          RFn         TA         TA    NaN  GdPrv
1458         NaN          Unf         TA         TA    NaN    NaN
1459         NaN          Fin         TA         TA    NaN    NaN

[1460 rows x 19 columns]
```

[6]:

```python
# 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

# one-hot encoder
categorical_transformer = Pipeline(steps=[
    ('imputer', SimpleImputer(strategy='constant',fill_value='missing')),
    ('onehot', OneHotEncoder(sparse=False,handle_unknown='ignore'))])

# ordinal encoder
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)])
```

[7]:
```
# fit_transform the training set
X_prep = preprocessor.fit_transform(X_train)
# little hacky, but collect feature names
feature_names = preprocessor.transformers_[0][-1] + \
                list(preprocessor.named_transformers_['cat'][1].
 ↪get_feature_names(cat_ftrs)) + \
                preprocessor.transformers_[2][-1]

df_train = pd.DataFrame(data=X_prep,columns=feature_names)
print(df_train.shape)

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

# transform  the holdout
df_holdout = preprocessor.transform(X_holdout)
df_holdout = pd.DataFrame(data=df_holdout,columns = feature_names)
print(df_holdout.shape)
```

```
(876, 221)
(292, 221)
(292, 221)
```

[8]:
```
df_train[ordinal_ftrs]
```

[8]:
```
     LotShape  Utilities  LandSlope  ExterQual  ExterCond  BsmtQual  BsmtCond  \
0         0.0        0.0        0.0        2.0        2.0       4.0       3.0
1         0.0        0.0        0.0        3.0        2.0       4.0       3.0
2         1.0        0.0        0.0        2.0        2.0       4.0       3.0
3         0.0        0.0        0.0        2.0        2.0       3.0       3.0
4         0.0        0.0        0.0        3.0        2.0       4.0       3.0
..        …         …         …         …         …        …       …
871       0.0        0.0        0.0        2.0        2.0       3.0       3.0
872       0.0        0.0        0.0        3.0        2.0       4.0       3.0
873       0.0        0.0        0.0        2.0        3.0       3.0       3.0
874       0.0        0.0        0.0        3.0        2.0       4.0       3.0
875       1.0        0.0        0.0        3.0        2.0       4.0       3.0

     BsmtExposure  BsmtFinType1  BsmtFinType2  HeatingQC  KitchenQual  \
```

```
0              1.0          1.0           1.0       4.0         2.0
1              3.0          6.0           1.0       4.0         3.0
2              3.0          5.0           2.0       3.0         3.0
3              1.0          4.0           1.0       2.0         2.0
4              1.0          6.0           1.0       4.0         3.0
..             …           …           …        …          …
871            1.0          3.0           1.0       2.0         2.0
872            1.0          1.0           1.0       4.0         3.0
873            1.0          1.0           1.0       2.0         2.0
874            2.0          1.0           1.0       3.0         4.0
875            1.0          1.0           1.0       4.0         3.0

     Functional  FireplaceQu  GarageFinish  GarageQual  GarageCond  PoolQC  \
0           7.0          0.0           2.0         3.0         3.0     0.0
1           7.0          4.0           2.0         3.0         3.0     0.0
2           7.0          0.0           2.0         3.0         4.0     0.0
3           7.0          2.0           2.0         3.0         3.0     0.0
4           7.0          0.0           2.0         3.0         3.0     0.0
..          …          …           …         …         …     …
871         7.0          0.0           1.0         3.0         3.0     0.0
872         7.0          0.0           2.0         3.0         3.0     0.0
873         5.0          0.0           2.0         3.0         3.0     0.0
874         7.0          4.0           2.0         3.0         3.0     0.0
875         7.0          4.0           2.0         3.0         3.0     0.0

     Fence
0      0.0
1      0.0
2      3.0
3      0.0
4      0.0
..     …
871    3.0
872    0.0
873    0.0
874    0.0
875    0.0

[876 rows x 19 columns]
```

1.4.3 2) Continuous features: mean or median imputation

- Imputation means you infer the missing values from the known part of the data
- sklearn’s SimpleImputer can do mean and median imputation
- USUALLY A BAD IDEA!
  - MCAR: mean/median of non-missing values is the same as the mean/median of the true underlying distribution, but the variances are different

- not MCAR: the mean/median and the variance of the completed dataset will be off
- supervised ML model is too confident (MCAR) or systematically off (not MCAR)

1.4.4 3) Exclude points or features with missing values

- easy to do with pandas
- it is an ACCEPTABLE approach under two conditions:
  - Little's test supports MCAR ($p > 0.05$)
  - only small fraction of points contain missing values (maybe a few percent?) OR the missing values are limited to one or a few features that can be dropped
- if the MCAR assumption is justified, dropping points will not introduce biases to your model
- due to the smaller sample size, the confidence of your model might suffer.
- what will you do with missing values when you deploy the model?

[9]:
```
print('data dimensions:',df_train.shape)
print('the p value of the mcar test:',mcar_test(df_train))
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])
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, 221)
the p value of the mcar test: 1.0
fraction of missing values in features:
LotFrontage    0.173516
MasVnrArea     0.004566
GarageYrBlt    0.050228
dtype: float64
fraction of points with missing values: 0.2237442922374429
```

[10]:
```
print(df_train.shape)
# by default, rows/points are dropped
df_r = df_train.dropna()
print(df_r.shape)
# drop features with missing values
df_c = df_train.dropna(axis=1)
print(df_c.shape)
```

```
(876, 221)
(680, 221)
(876, 218)
```

1.5 Learning Objectives

By the end of this workshop, you will be able to - Describe the three main types of missingness patterns - Evaluate simple approaches for handling missing values - **Apply XGBoost to a dataset with missing values** - Apply multivariate imputation - Apply the reduced-features model (also called the pattern submodel approach) - Decide which approach is best for your dataset

1.6 XGBoost and missing values

- sklearn raises an error if the feature matrix (X) contains nans.
- XGBoost doesn't!
- If a feature with missing values is split:
  - XGBoost tries to put the points with missing values to the left and right
  - calculates the impurity measure for both options
  - puts the points with missing values to the side with the lower impurity
- if missingness correlates with the target variable, XGBoost extracts this info!

[11]:
```
import xgboost
from sklearn.model_selection import ParameterGrid
from sklearn.metrics import mean_squared_error

param_grid = {"learning_rate": [0.03],
              "n_estimators": [2000],
              "seed": [0],
              #"n_jobs": [-1],
              #"reg_alpha": [0e0,0.1,0.31622777,1.,3.16227766,10.],
              #"reg_lambda": [0e0,0.1,0.31622777,1.,3.16227766,10.],
              "missing": [np.nan],
              #"max_depth": [1,2,3,4,5],
              "colsample_bytree": [0.9],
              "subsample": [0.66]}

XGB = xgboost.XGBRegressor()
XGB.set_params(**ParameterGrid(param_grid)[0])
XGB.fit(df_train,y_train,early_stopping_rounds=50,eval_set=[(df_test, y_test)],␣
 ↪verbose=False)
print('the test RMSE:',XGB.evals_result()['validation_0']['rmse'][-1])
y_holdout_pred = XGB.predict(df_holdout)
print('the holdout RMSE:',np.sqrt(mean_squared_error(y_holdout,y_holdout_pred)))
```

```
the test RMSE: 23486.925781
the holdout RMSE: 31748.96283078089
```

1.7 Learning Objectives

By the end of this workshop, you will be able to - Describe the three main types of missingness patterns - Evaluate simple approaches for handling missing values - Apply XGBoost to a dataset with missing values - **Apply multivariate imputation** - Apply the reduced-features model (also called the pattern submodel approach) - Decide which approach is best for your dataset

1.8 Multivariate Imputation

- models each feature with missing values as a function of other features
  - at each step, a feature with nans is designated as target variable y and the other features are treated as feature matrix X
  - a regressor is trained on (X, y) for known y

  - then, the regressor is used to predict the missing values of y
- in the ML pipeline:
  - create n imputed datasets
  - run all of them through the ML pipeline
  - generate n holdout scores
  - the uncertainty in the holdout scores is due to the uncertainty in imputation
- works on MCAR and MAR, fails on MNAR
- paper here

2 sklearn's IterativeImputer

[12]:
```
from sklearn.experimental import enable_iterative_imputer
from sklearn.impute import IterativeImputer
from sklearn.ensemble import RandomForestRegressor

print(df_train[['LotFrontage','MasVnrArea','GarageYrBlt']].head())

imputer = IterativeImputer(estimator = RandomForestRegressor(n_estimators=10),␣
 ↪random_state=0)
X_impute = imputer.fit_transform(df_train)
df_train_imp = pd.DataFrame(data=X_impute, columns = df_train.columns)

print(df_train_imp[['LotFrontage','MasVnrArea','GarageYrBlt']].head())

df_test_imp = pd.DataFrame(data=imputer.transform(df_test), columns = df_train.
 ↪columns)
df_holdout_imp = pd.DataFrame(data=imputer.transform(df_holdout), columns =␣
 ↪df_train.columns)
```

```
   LotFrontage  MasVnrArea  GarageYrBlt
0     0.424926   -0.573303     0.979398
1          NaN    0.492835     1.018748
2          NaN   -0.573303     0.192399
3    -0.049970    0.810076    -0.476551
4    -1.474659   -0.022031     0.979398
   LotFrontage  MasVnrArea  GarageYrBlt
0     0.424926   -0.573303     0.979398
1    -1.289018    0.492835     1.018748
2    -0.287418   -0.573303     0.192399
3    -0.049970    0.810076    -0.476551
4    -1.474659   -0.022031     0.979398

/Users/azsom/opt/anaconda3/envs/data1030/lib/python3.7/site-
packages/sklearn/impute/_iterative.py:670: ConvergenceWarning:
[IterativeImputer] Early stopping criterion not reached.
  " reached.", ConvergenceWarning)
```

[13]:
```
XGB.fit(df_train_imp,y_train,early_stopping_rounds=50,eval_set=[(df_test_imp,␣
 ↪y_test)], verbose=False)
print('the test RMSE:',XGB.evals_result()['validation_0']['rmse'][-1])
y_holdout_pred = XGB.predict(df_holdout_imp)
print('the holdout RMSE:',np.sqrt(mean_squared_error(y_holdout,y_holdout_pred)))
```

```
the test RMSE: 23189.175781
the holdout RMSE: 32290.240629124994
```

2.1 Learning Objectives

By the end of this workshop, you will be able to - Describe the three main types of missingness patterns - Evaluate simple approaches for handling missing values - Apply XGBoost to a dataset with missing values - Apply multivariate imputation - **Apply the reduced-features model (also called the pattern submodel approach)** - Decide which approach is best for your dataset

2.2 Reduced-features model (or pattern submodel approach)

- first described in 2007 in a JMLR article as the reduced features model
- in 2018, "rediscovered" as the pattern submodel approach in Biostatistics

My holdout set:

index	feature 1	feature 2	feature 3	target var
0	NA	45	NA	0
1	NA	NA	8	1
2	12	6	34	0
3	1	89	NA	0
4	0	NA	47	1
5	687	24	67	1
6	NA	23	NA	1

To predict points 0 and 6, I will use train and test points that are complete in feature 2.

To predict point 1, I will use train and test points that are complete in feature 3.

To predict point 2 and 5, I will use train and test points that are complete in features 1-3.

Etc. We will train as many models as the number of patterns in holdout.

2.3 How to determine the patterns?

[14]:
```
mask = df_holdout[['LotFrontage','MasVnrArea','GarageYrBlt']].isnull()
unique_rows, counts = np.unique(mask, axis=0,return_counts=True)
print(unique_rows.shape) # 6 patterns, we will train 6 models
for i in range(len(counts)):
    print(unique_rows[i],counts[i])
```

```
(6, 3)
```

```
[False False False] 223
[False False  True] 21
[False  True False] 1
[ True False False] 44
[ True False  True] 2
[ True  True False] 1
```

[15]:

```python
def xgb_model(X_train, Y_train, X_test, Y_test, X_holdout, Y_holdout,␣
 ↪verbose=1):

    # make into row vectors to avoid an obnoxious sklearn/xgb warning
    Y_train = np.reshape(np.array(Y_train), (1, -1)).ravel()
    Y_test = np.reshape(np.array(Y_test), (1, -1)).ravel()
    Y_holdout = np.reshape(np.array(Y_holdout), (1, -1)).ravel()

    XGB = xgboost.XGBRegressor(n_jobs=1)

    # find the best parameter set
    param_grid = {"learning_rate": [0.03],
                  "n_estimators": [2000],
                  "seed": [0],
                  #"n_jobs": [6],
                  #"reg_alpha": [0e0,0.1,0.31622777,1.,3.16227766,10.],
                  #"reg_lambda": [0e0,0.1,0.31622777,1.,3.16227766,10.],
                  "missing": [np.nan],
                  #"max_depth": [1,2,3,4,5],
                  "colsample_bytree": [0.9],
                  "subsample": [0.66]}

    pg = ParameterGrid(param_grid)

    scores = np.zeros(len(pg))

    for i in range(len(pg)):
        if verbose >= 5:
            print("Param set " + str(i + 1) + " / " + str(len(pg)))
        params = pg[i]
        XGB.set_params(**params)
        eval_set = [(X_test, Y_test)]
        XGB.fit(X_train, Y_train,
                early_stopping_rounds=50, eval_set=eval_set, verbose=False)#␣
 ↪with early stopping
        Y_test_pred = XGB.predict(X_test, ntree_limit=XGB.best_ntree_limit)
        scores[i] = mean_squared_error(Y_test,Y_test_pred)

    best_params = np.array(pg)[scores == np.max(scores)]
    if verbose >= 4:
```

```
        print('Test set max score and best parameters are:')
        print(np.max(scores))
        print(best_params)

    # test the model on the holdout set with best parameter set
    XGB.set_params(**best_params[0])
    XGB.fit(X_train,Y_train,
            early_stopping_rounds=50,eval_set=eval_set, verbose=False)
    Y_holdout_pred = XGB.predict(X_holdout, ntree_limit=XGB.best_ntree_limit)

    if verbose >= 1:
        print ('The MSE is:',mean_squared_error(Y_holdout,Y_holdout_pred))
    if verbose >= 2:
        print ('The predictions are:')
        print (Y_holdout_pred)
    if verbose >= 3:
        print("Feature importances:")
        print(XGB.feature_importances_)

    return (mean_squared_error(Y_holdout,Y_holdout_pred), Y_holdout_pred, XGB.
 ↪feature_importances_)

# Function: Reduced-feature XGB model
# all the inputs need to be pandas DataFrame
def reduced_feature_xgb(X_train, Y_train, X_test, Y_test, X_holdout, Y_holdout):

    # find all unique patterns of missing value in holdout set
    mask = X_holdout.isnull()
    unique_rows = np.array(np.unique(mask, axis=0))
    all_Y_holdout_pred = pd.DataFrame()

    print('there are', len(unique_rows), 'unique missing value patterns.')

    # divide holdout sets into subgroups according to the unique patterns
    for i in range(len(unique_rows)):
        print ('working on unique pattern', i)
        ## generate X_holdout subset that matches the unique pattern i
        sub_X_holdout = pd.DataFrame()
        sub_Y_holdout = pd.Series()
        for j in range(len(mask)): # check each row in mask
            row_mask = np.array(mask.iloc[j])
            if np.array_equal(row_mask, unique_rows[i]): # if the pattern␣
 ↪matches the ith unique pattern
                sub_X_holdout = sub_X_holdout.append(X_holdout.iloc[j])# append␣
 ↪the according X_holdout row j to the subset
                sub_Y_holdout = sub_Y_holdout.append(Y_holdout.iloc[[j]])#␣
 ↪append the according Y_holdout row j
```

```
        sub_X_holdout = sub_X_holdout[X_holdout.columns[~unique_rows[i]]]

        ## choose the according reduced features for subgroups
        sub_X_train = pd.DataFrame()
        sub_Y_train = pd.DataFrame()
        sub_X_test = pd.DataFrame()
        sub_Y_test = pd.DataFrame()
        # 1.cut the feature columns that have nans in the according␣
↪sub_X_holdout
        sub_X_train = X_train[X_train.columns[~unique_rows[i]]]
        sub_X_test = X_test[X_test.columns[~unique_rows[i]]]
        # 2.cut the rows in the sub_X_train and sub_X_test that have any nans
        sub_X_train = sub_X_train.dropna()
        sub_X_test = sub_X_test.dropna()
        # 3.cut the sub_Y_train and sub_Y_test accordingly
        sub_Y_train = Y_train.iloc[sub_X_train.index]
        sub_Y_test = Y_test.iloc[sub_X_test.index]

        # run XGB
        sub_Y_holdout_pred = xgb_model(sub_X_train, sub_Y_train, sub_X_test,
                                       sub_Y_test, sub_X_holdout,␣
↪sub_Y_holdout, verbose=0)
        sub_Y_holdout_pred = pd.
↪DataFrame(sub_Y_holdout_pred[1],columns=['sub_Y_holdout_pred'],
                                          index=sub_Y_holdout.index)
        print('    RMSE:',np.
↪sqrt(mean_squared_error(sub_Y_holdout,sub_Y_holdout_pred)))
        # collect the holdout predictions
        all_Y_holdout_pred = all_Y_holdout_pred.append(sub_Y_holdout_pred)

    # rank the final Y_holdout_pred according to original Y_holdout index
    all_Y_holdout_pred = all_Y_holdout_pred.sort_index()
    Y_holdout = Y_holdout.sort_index()

    # get global RMSE
    total_RMSE = np.sqrt(mean_squared_error(Y_holdout,all_Y_holdout_pred))

    return total_RMSE
```

2.3.1 A python implementation is available on the skipped slide

[16]:
```
print('final RMSE:',reduced_feature_xgb(df_train, y_train, df_test, y_test,␣
↪df_holdout, y_holdout))
```

```
there are 6 unique missing value patterns.
working on unique pattern 0
```

```
/Users/azsom/opt/anaconda3/envs/data1030/lib/python3.7/site-
packages/ipykernel_launcher.py:76: DeprecationWarning: The default dtype for
empty Series will be 'object' instead of 'float64' in a future version. Specify
a dtype explicitly to silence this warning.
```

```
   RMSE: 35277.53669207676
working on unique pattern 1
```

```
/Users/azsom/opt/anaconda3/envs/data1030/lib/python3.7/site-
packages/ipykernel_launcher.py:76: DeprecationWarning: The default dtype for
empty Series will be 'object' instead of 'float64' in a future version. Specify
a dtype explicitly to silence this warning.
```

```
   RMSE: 11607.857261825593
working on unique pattern 2
```

```
/Users/azsom/opt/anaconda3/envs/data1030/lib/python3.7/site-
packages/ipykernel_launcher.py:76: DeprecationWarning: The default dtype for
empty Series will be 'object' instead of 'float64' in a future version. Specify
a dtype explicitly to silence this warning.
```

```
   RMSE: 1134.5625
working on unique pattern 3
```

```
/Users/azsom/opt/anaconda3/envs/data1030/lib/python3.7/site-
packages/ipykernel_launcher.py:76: DeprecationWarning: The default dtype for
empty Series will be 'object' instead of 'float64' in a future version. Specify
a dtype explicitly to silence this warning.
```

```
   RMSE: 18366.394043603428
working on unique pattern 4
```

```
/Users/azsom/opt/anaconda3/envs/data1030/lib/python3.7/site-
packages/ipykernel_launcher.py:76: DeprecationWarning: The default dtype for
empty Series will be 'object' instead of 'float64' in a future version. Specify
a dtype explicitly to silence this warning.
```

```
   RMSE: 18521.340554971906
working on unique pattern 5
```

```
/Users/azsom/opt/anaconda3/envs/data1030/lib/python3.7/site-
packages/ipykernel_launcher.py:76: DeprecationWarning: The default dtype for
empty Series will be 'object' instead of 'float64' in a future version. Specify
a dtype explicitly to silence this warning.
```

```
   RMSE: 65343.46875
final RMSE: 32061.23877235819
```

2.4 Learning Objectives

By the end of this workshop, you will be able to - Describe the three main types of missingness patterns - Evaluate simple approaches for handling missing values - Apply XGBoost to a dataset with missing values - Apply multivariate imputation - Apply the reduced-features model (also called the pattern submodel approach) - **Decide which approach is best for your dataset**

2.5 Which approach is best for my data?

- **XGB**: run n XGB models with n different seeds
- **imputation**: prepare n different imputations and run n XGB models on them
- **reduced-features**: run n reduced-features model with n different seeds
- rank the three methods based on how significantly different the corresponding mean scores are

Now you can - Describe the three main types of missingness patterns - Evaluate simple approaches for handling missing values - Apply XGBoost to a dataset with missing values - Apply multivariate imputation - Apply the reduced-features model (also called the pattern submodel approach) - Decide which approach is best for your dataset

#

Thanks for your attention!