Week1

- Big picture
  - What are the inputs and outputs? Single or multiple?
  - What's the business objective?
  - Algo selection – Supervised-Unsupervised-RL, Regression-Classification, Continuous learning-periodic updates, Batch-Online
  - Select performance measure – Regression (MSE-MAE), Classification (Precision-Recall-F1-Score-Accuracy)
  - What is the current solution? Provides for a useful baseline
- Get the data
  - Spread about multiple tables, files, documents available locally, or on the web.
  - Structured-Unstructured data.
  - Understand the data and its statistics – `info()` and `describe()`
  - Distribution of examples by features/label. Use a histogram.
  - Create test set using `train_test_split()` in order to avoid data snooping bias. Used to select k% data for test-set
  - `train_test_split()` may be used to process multiple datasets with an identical number of rows and select the same indices from these datasets. Useful when labels are in different dataframes.
  - Alternatively, use stratified sampling to divide the population into homogeneous groups called strata and sample data from each strata representative of overall distribution. Use `StrafifiedShuffleSplit.split()` to divide data between train and test.

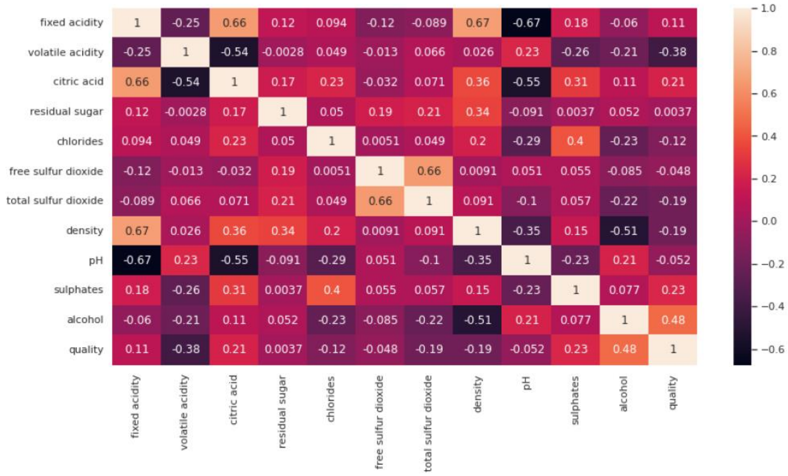
```
from sklearn.model_selection import StratifiedShuffleSplit
split = StratifiedShuffleSplit(n_splits=1, test_size=0.2, random_state=42)
for train_index, test_index in split.split(data, data["quality"]):
  strat_train_set = data.loc[train_index]
  strat_test_set = data.loc[test_index]
```

- Visualize the data.
  - Enables to understand features and their relationship among themselves and with the output label.
  - Commonly used metric is standard correlation coefficient {-1, 1} to measure correlation among features.

```
corr_matrix = exploration_set.corr()
```

  - Correlation coefficient can capture only linear relationship; use rank correlation, for non-linear relationship.
  - Use heatmap to visualize correlation matrix.

```
plt.figure(figsize=(14,7))
sns.heatmap(corr_matrix, annot=True)
```



- Note that correlation coefficient on the diagonal is 1.
- Darker colors (black) are used to represent negative correlations, while fainter colors are used to denote positive correlations.
- Alternatively use a scatter matrix to visualize correlation.

- Pre-processing data
  - Problems with data includes outliers, missing values, different scales, non-numeric attributes, non-amenable distribution of data.
  - Use `isna().sum()` to find out if there are missing values. In case there are missing values, use `SimpleImputer` (with appropriate strategy like mean-median) or Standard to fill them up. However, make sure that non-numerical values are dropped before applying imputing step.

```
from sklearn.impute import SimpleImputer
imputer = SimpleImputer(strategy="median")

imputer.fit(wine_features)

tr_features = imputer.transform(wine_features)
```

  - Alternatively, you can drop the corresponding row using dropna() or drop()
  - Convert categories to numbers using `OrdinalEncoder` or `OneHotEncoder`
  - Use `MinMaxScaler` or `StandardScaler` for feature scaling.
  - `MinMaxScaler` fits every feature into a range [0, 1]
  - `StandardScaler` is less affected by outliers than `MinMaxScaler`.
  - Scaling techniques should be *learnt* with on the training data, and can be used to transform the training and test data.
  - Pipelines are typically used to perform operations sequentially. The pipeline exposes the same method as the final estimator.

```
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import StandardScaler
transform_pipeline = Pipeline([
                              ('imputer', SimpleImputer(strategy="median")),
                              ('std_scaler', StandardScaler()),])
wine_features_tr = transform_pipeline.fit_transform(wine_features)
```

  - Here, the pipeline first performs imputation of missing values using `SimpleImputer` (with a 'median' strategy) and its result is passed for standardization.
  - Pipelines only work with one type of data. Use `ColumnTransformer` to work with columns of different types.

- Select and train ML model
    - Build a quick base-line model. Evaluate the performance on training as well as test sets, using `mean_squared_error(), mean_absolute_error(), r2_score()` etc.
    - We can use a cross-validation for robust performance of model performance, where multiple validation sets are created from the training set. This process generates a separate MSE for each validation set. We can use the mean/std.deviation of all such MSEs to evaluate the performance.
    - It's a good practice to build a few quick models without tuning hyperparameters and shortlist a few promising models among them, and work on them further.
    - In case of underfitting, use model with more capacity and use less constraints/regularization.
    - In case of overfitting, use more data, a simpler model, and use more constraints/regularization.
    - In order to find the best combination of hyper-parameters, use `GridSearchCV or RandomizedSearchCV`, both of which build multiple models with different sets of hyper-parameters.
    - Utilize the `param_grid` to work with all combinations of these parameter values. For example, in order to select the best combination for a `RandomForest` regressor, you may use the following `param_grid`.

    ```
    param_grid = [
     {'n_estimators': [3, 10, 30], 'max_features': [2, 4, 6, 8]},
     {'bootstrap': [False], 'n_estimators': [3, 10], 'max_features': [2, 3, 4]},
    ]
    ```

    In the above case, the first dictionary yields 12 combinations and second dictionary yields 6 combinations, thus resulting in 18 total combinations.
    - The models could be built in parallel, by setting parameter *n_jobs* to -1.
    - Set parameter *error_score* to 0, if you do not want the process to stop when one of the models fails to build for any reason.
    - Find the best parameter set and the best model resulting from the process using `best_params_` and `best_estimator_` attributes respectively.
    - Setting parameter *refit* to True, retrains the best estimator (found using `best_estimator_` property) on the full training set, so as to improve upon the model again. Note that the original test set is not used in the process.
    - `GridSearchCV` can prove costly when the hyperparameter space is quite large. In such cases, use `RandomizedSearchCV.`
    - `RandomizedSearchCV` selects a random value for each hyperparameter at the start of each iteration and repeats the process for *n_iter* random combinations.
    - In the case of `GridSearchCV/RandomizedSearchCV, best_estimator_.feature_importances_`property will allows to selectively drop features based on their importances.
    - Apart from the above two generic cross-validation methods, certain models have more specialized methods for cross-validation. Examples include `LassoCV, RidgeCV, ElasticNetCV`
    - Once the predictions are made on the test set, it's a good idea to get 95% confidence internal of the evaluation metric.

```
from scipy import stats
confidence = 0.95
squared_errors = (quality_test_predictions - wine_labels_test) ** 2
stats.t.interval(confidence, len(squared_errors) - 1,
                 loc=squared_errors.mean(),
                 scale=stats.sem(squared_errors))
```

```
(0.29159276569581916, 0.4153100120819586)
```

- Present your solution
  - Document everything
  - Create clear visualizations.
- Launch, monitor and maintain your system
  - System outages
  - Degradation of model performance.
  - Manual evaluations
  - Regular assessments on data quality

Data loading mechanisms

- The dataset loaders (load_*) are used to load toy datasets bundled with sklearn.
- The dataset fetchers (fetch_*) are used to download and load datasets from the internet.
- The dataset generators (make_*) are used to generate controlled synthetic datasets.
- Both loaders and fetchers return a Bunch object, which is a dictionary with two keys `data` and `target`. There could be additional keys like `feature_names`, `target_names`, `DESCR` and `filename`
- Generators return a tuple contains the `data` and `target`.
- Loaders and fetchers can also return tuple (like in the case of generators), if `return_X_y` is set to True.
- `make_regression()` produces regression datasets.

  `X, y = make_regression(n_samples=100, n_features=5, n_targets=1, shuffle=True, random_state=42)` # Generates single label regression data.

  `X, y = make_regression(n_samples=100, n_features=5, n_targets=5, shuffle=True, random_state=42)` # Generates multiple label regression data
- `make_blobs()` and `make_classification()` creates a bunch of normally-distributed clusters of points and then assign one or more clusters to each class thereby creating multi-class datasets.

  `X, y = make_blobs(n_samples=10, centers=3, n_features=2, random_state=42)` # Generates 3 clusters. Used in unsupervised ML

  `X, y = make_classification(n_samples=100, n_features=10, n_classes=2, n_clusters_per_class=1, random_state=42)` # Generates multiple classes. Also generates clusters per classes.
- `make_multilabel_classification()` generates multi-label datasets.

  `X, y = make_multilabel_classification(n_samples=100, n_features=20, n_classes=5, n_labels=2)`

  Note that `n_labels` represents the average number of labels in each example.

Week2

- Typically pre-processing includes dealing with
  - missing values in features, (`sklearn.impute`)

- scaling features (`sklearn.preprocessing`)
- converting categorial features to numerical representation (`sklearn.preprocessing`)
- extracting features from non-numeric data (`sklearn.feature_extraction`)
- reducing too many features (`sklearn.decomposition.pca`)
- expanding the features (`sklearn.kernel_approxiation`)

- It's important to apply the same pre-processing method to the train, test and eval sets. Hence, it's best to use pipelines with appropriate transformations.

Feature extraction

- APIs typically used for feature extraction from data are
  - `DictVectorizer` # Converts original data in dictionary format to a matrix.

    Example: `DictVectorizer` transforms

    ```
    data =
    [{'age': 4, 'height':96.0},
    {'age': 1, 'height':73.9},
    {'age': 3, 'height':88.9},
    {'age': 2, 'height':81.6}]
    ```

    into $\begin{bmatrix} 4 & 96.0 \\ 1 & 73.9 \\ 3 & 88.9 \\ 2 & 81.6 \end{bmatrix}$
  - `FeatureHasher` # Outputs a sparse matrix, by applying a hash function to the features to determine the column index in the resultant matrix. `FeatureHasher` is a high-speed and low-memory vectorizer
- In addition, features can also be extracted from images and text using APIs built into the same module.

Imputing data

- `SimpleImputer` – uses one of the strategies *mean, median, most_frequent, constant* to impute

  Example: `SimpleImputer` with a mean strategy transforms $\begin{bmatrix} 7 & 1 \\ nan & 8 \\ 2 & nan \\ 9 & 6 \end{bmatrix}$ into $\begin{bmatrix} 7 & 1 \\ 6 & 8 \\ 2 & 5 \\ 9 & 6 \end{bmatrix}$
- `KNNImputer` – Find `n_neighbors` nearest neighbors based on Euclidean distance and uses mean on these datapoints to impute.

  In the presence of missing coordinates, the Euclidean distance is calculated by ignoring the missing values and scaling up the weight of the non-missing coordinates.

  $$d_{xy} = \sqrt{weight \ * squared\ distance\ from\ present\ coordinates}$$

  where,

  $$weight = \frac{Total\ number\ of\ coordinates}{Number\ of\ present\ coordinates}$$

  For example, the Euclidean distances between two points (3, **NA**, 5) and (1, 0, 0) is:

  $$\sqrt{\frac{3}{2}\{(3-1)^2 + (5-0)^2\}} = 6.595453$$

  Example: KNNImputer with 2 neighbors transforms $\begin{bmatrix} 1. & 2. & nan. \\ 3. & 4. & 3. \\ nan & 6. & 5. \\ 8. & 8. & 7. \end{bmatrix}$ into $\begin{bmatrix} 1. & 2. & 4. \\ 3. & 4. & 3. \\ 5.5 & 6. & 5. \\ 8. & 8. & 7. \end{bmatrix}$
- While imputing, presence of missing values can be indicated by using the `MissingIndicator` API

Feature scaling

- APIs used are

- `StandardScaler` # $\mathbf{x}' = \frac{\mathbf{x}-\mu}{\sigma}$. Example: `StandardScaler` Transforms $\begin{bmatrix} 4 \\ 3 \\ 2 \\ 5 \\ 6 \end{bmatrix}$ into $\begin{bmatrix} 0 \\ -1/\sqrt{2} \\ -2/\sqrt{2} \\ 1/\sqrt{2} \\ 2/\sqrt{2} \end{bmatrix}$
- `MaxAbsScaler` # $\mathbf{x}' = \frac{\mathbf{x} - \mathbf{x}.min}{\mathbf{x}.max - \mathbf{x}.min}$. Example: `MaxAbsScaler` Transforms $\begin{bmatrix} 15 \\ 2 \\ 5 \\ -2 \\ -5 \end{bmatrix}$ into $\begin{bmatrix} 1 \\ 0.35 \\ 0.5 \\ 0.6 \\ 0 \end{bmatrix}$
- `MinMaxScaler` # $\mathbf{x}' = \frac{\mathbf{x}}{\mathrm{MaxAbsoluteValue}}$, where $\mathrm{MaxAbsoluteValue} = \max(\mathbf{x}.max, |\mathbf{x}.min|)$
  Note that the resultant values fall within range [-1,1]

  Example: `MinMaxScaler` transforms $\begin{bmatrix} 4 \\ 2 \\ 5 \\ -2 \\ -100 \end{bmatrix}$ into $\begin{bmatrix} 0.04 \\ 0.02 \\ 0.05 \\ -0.02 \\ -1 \end{bmatrix}$

Other transformers

- `FunctionTransformer` applies user defined function on dataset in order to transform.

  Example: `log2` transforms $\begin{bmatrix} 128 & 2 \\ 2 & 256 \\ 4 & 1 \\ 512 & 64 \end{bmatrix}$ into $\begin{bmatrix} 7 & 1 \\ 1 & 8 \\ 2 & 0 \\ 9 & 6 \end{bmatrix}$
- `PolynomialFeatures` are used to add complex features to the dataset.

  Example: `PolynomialFeatures` with degree-3 transforms $\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2]$ into $\mathbf{X}' = [\mathbf{x}_1, \mathbf{x}_2,\ \mathbf{x}_1\mathbf{x}_2,\ \mathbf{x}_1^2,\ \ \mathbf{x}_2^2,\ \mathbf{x}_1^2\mathbf{x}_2,\ \mathbf{x}_1\mathbf{x}_2^2,\ \mathbf{x}_1^3,\ \mathbf{x}_2^3]$
- `KBinsDiscretizer` divides a continuous variables into bins, and applies one-hot/ordinal encoding to the bin labels.

  Example: `KBinsDiscretizer` using 5 bins transforms $\begin{bmatrix} 0 \\ 0.125 \\ 0.25 \\ 0.375 \\ 0.5 \\ 0.675 \\ 0.75 \\ 0.875 \\ 1.0 \end{bmatrix}$ into $\begin{bmatrix} 0. \\ 0. \\ 1. \\ 1. \\ 2. \\ 3. \\ 3. \\ 4. \\ 4. \end{bmatrix}$
- `OneHotEncoder` creates columns equal to the unique number of inputs in the column. Each column has a 1 in it and rest have 0.

  Example: `OneHotEncoder` transforms $\begin{bmatrix} 1 \\ 2 \\ 3 \\ 1 \end{bmatrix}$ into $\begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$
- `LabelEncoder` encodes target labels with value from 0 and K-1, where K is the number of unique values.

  Example: `LabelEncoder` transforms $\begin{bmatrix} 1 \\ 2 \\ 6 \\ 1 \\ 8 \\ 6 \end{bmatrix}$ into $\begin{bmatrix} 0 \\ 1 \\ 2 \\ 0 \\ 3 \\ 2 \end{bmatrix}$
- `OrdinalEncoder` encodes categorical features with value from 0 and K-1, where K is the number of unique values. Note that `OrdinalEncoder` can operate multi dimensional data, while `LabelEncoder` can transform only 1D data.

Example: `OrdinalEncoder` transforms $\begin{bmatrix} 1 & \text{‘male’} \\ 2 & \text{‘female’} \\ 6 & \text{‘female’} \\ 1 & \text{‘male’} \\ 8 & \text{‘male’} \\ 6 & \text{‘female’} \end{bmatrix}$ into $\begin{bmatrix} 0 & 1 \\ 1 & 0 \\ 2 & 0 \\ 0 & 1 \\ 3 & 1 \\ 2 & 0 \end{bmatrix}$

- `LabelBinarizer` creates columns equal to the unique number of inputs in the column. Each column has a 1 in it and rest have 0. Functionally, it's similar to `OneHotEncoder`, but `LabelBinarizer` is preferred on labels, while `OneHotEncoder` is preferred on features.

  Example: `OrdinalEncoder` transforms $\begin{bmatrix} 1 \\ 2 \\ 6 \\ 1 \\ 8 \\ 6 \end{bmatrix}$ into $\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$
- `MultiLabelBinarizer` creates columns equal to the unique number of inputs in the column. It's similar to `LabelBinarizer`, but for multiple labels. Thus, multiple columns can have 1 in the output.

  Example: `MultiLabelBinarizer transforms` movie_genres = [{'action', 'comedy' }, {'comedy'}, {'action', 'thriller'}, {'science-fiction', 'action', 'thriller'}] to $\begin{bmatrix} 1 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 1 \end{bmatrix}$
- `add_dummy_feature` is not a transformer as such; augments the dataset with a column vector, each of whose value is `1.`

  Example: Using this function on $\begin{bmatrix} 7 & 1 \\ 1 & 8 \\ 2 & 0 \\ 9 & 6 \end{bmatrix}$ results in $\begin{bmatrix} 1 & 7 & 1 \\ 1 & 1 & 8 \\ 1 & 2 & 0 \\ 1 & 9 & 6 \end{bmatrix}$

Feature Selection

- Helps at removing features that do not contribute significantly towards the model, thus leading to a decrease in dataset size and hence the computation cost.
- Filter methods:
  - `VarianceThreshold` removes all features with variance below a certain threshold. By default, the threshold is 0.
  - `SelectKBest` removes all, but the k highest-scoring features
  - `SelectPercentile` removes all, but the highest-scoring k% of features
  - `GenericUnivariateSelect` offers a generic approach for the above features, by setting *mode* to one of 'percentile', 'k_best', 'fpr', 'fdr', 'fwe'
  - `SelectFpr` selects features based on a false positive test rate.
  - `SelectFdr` selects features beased on an estimated false discovery rate
  - `SelectFwe` selects features based on family-wise error rate
- Wrapper methods:
  - `RFE` removes features recursively until the desired number of features are reached.
  - `RFECV` uses cross-validation to achieve the same output as RFE
  - `SelectFromModel` selects features based on `coef_` and `feature_importances_` from the trained estimator
  - `SequentialFeatureSelector` selects by either *forward selection* or *backward selection*. Note that changing the direction could typically yield different results.

- Each of the above APIs can use one of the scoring functions from
  - Mutual Information: `mutual_info_regression, mutual_info_classif`
    NOTE: Non-negative. Higher value indicates higher dependency. 0 indicates independence.
  - Chi-square: `chi2` (can be used only for classification problems)
    NOTE: Calculate between frequency of occurrence (of a feature) and label. Higher value indicates higher dependency.
  - F-statistics: `f_regression, f_classif`

  NOTE: Mutual Information and Chi-square are recommended for sparse data.

- `ColumnTransformer` helps transform heterogenous data by applying different transformers to separate subsets of features.
  Example:
  ```
  column_trans = ColumnTransformer(
      [('ageScaler', CountVectorizer(), [0]]),
       ('genderEncoder', OneHotEncoder(dtype='int'), [1])],
      remainder='drop', verbose_feature_names_out=False)
  ```
  applies `CountVectorizer` on column0 and `OneHotEncoder` to column1 of the dataset.
- `TransformedTargetRegression` helps regress on some complicated function y, and return its inverse during predict.
- `sklearn.decomposition.PCA` is used to project the feature matrix or data to a lower dimensional space, by capturing bulk of the variance in as few directions as possible.
- It is important to apply exactly same transformation on training, evaluation and test set in the same order.
  Example:
  ```
  si = SimpleImputer()
  X_imputed = si.fit_transform(X)
  ss =StandardScaler()
  X_scaled = ss.fit_transform(X_imputed)
  ```
- Alternatively, use `Pipeline` and `FeatureUnion`.
  - `Pipeline` constructs a chain of multiple transformers to execute a fixed sequence of steps in data preprocessing and modelling. Each step must be a tuple of (Step name, sklearn API, and optionally a list of the column numbers).
    Example:
    ```
    estimators = [
      ('simpleImputer', SimpleImputer()),
      ('standardScaler', StandardScaler()),
    ]
    pipe = Pipeline(steps=estimators)
    pipe.fit_transform(X)
    ```
  - `FeatureUnion` combines output from several transformer objects by creating a new transformer from them.
    Example:
    ```
    num_pipeline = Pipeline([('selector',ColumnTransformer([('select_first_4',
                                                              'passthrough',
                                                              slice(0,4))])),
                             ('imputer', SimpleImputer(strategy="median")),
                             ('std_scaler', StandardScaler()),
                            ])
    cat_pipeline = ColumnTransformer([('label_binarizer', LabelBinarizer(),[4]),
                                     ])
    full_pipeline = FeatureUnion(transformer_list=
                                 [("num_pipeline", num_pipeline),
                                  ("cat_pipeline", cat_pipeline),])
    ```

- Note that the intermediate steps of a `Pipeline` must implement `fit` and `transform`, whereas the final estimator only needs to implement `fit`.
- Each step in the pipeline can be accessed using a 0-based index. Thus in the above example, pipe[-1] refers to the `StandardScaler()`
- In order to access the parameters for each step, use the format <step_name>__<parameter name>

  Example:
```
estimators = [
  ('simpleImputer', SimpleImputer()),
  ('pca', PCA()),
  ('regressor', LinearRegression())
]
pipe = Pipeline(steps=estimators)

pipe.set_params(pca__n_components = 2)
```
- Transformers can be cached by setting `memory` parameter in the `Pipeline` object.
- `GridSearchCV` may be applied on the pipeline in order to cross-validate with specific hyper-parameters for each step.

Week3

- Use `DummyRegressor` with an appropriate strategy (mean, median, quantile, constant) to develop a baseline regressor model. Note that the strategy is based on some statistic property of the training set or a user-specified value.

SGDRegressor

- Typically used in a large training setup with greater than 10K samples. For smaller training sets, use `Ridge` or `Lasso`
- The advantage of Lasso is its efficiency, which is basically linear in the number of training examples.
- Provides greater control on the optimization process through its hyperparameters
  - *loss* (squared_error, huber)
  - *penalty* (l1, l2, elasticnet)
  - *learning_rate* (constant, optimal, invscaling, adaptive). Default is *invscaling*.
  - *early_stopping* (True, False)
- If *learning_rate* is set to *invscaling,* it reduces after every iteration as $\eta^{(t)} = \frac{\eta_0}{t^{power\_t}}$ Note that *eta0* and *power_t* are both hyperparameters.
- If *learning_rate* is set to *adaptive,* it is kept to the initial value as long as the training loss reduces, and gets divided by an arbitrary number (5) when the stopping criterion is reached. The algorithm stops when the learning rate goes below 10^{-6}
- Stopping criterion occurs when the training loss doesn't improve (loss > best_loss – *tol*) for *n_iter_no_change* consecutive epochs. Alternatively, the algorithm stops when the validation score (as suggested by the parameter *scoring*) doesn't improve by at least *tol* for *n_iter_no_change* consecutive epochs, as far as *early_stopping* is set to True and *validation_fraction* is set. By default, the algorithm stops after reaching *max_iter* in both cases.
- `SGDRegressor` is very sensitive to feature scaling, so it highly recommended to scale the input feature matrix, before its's fit to the data.

- Training data can be shuffled after each epoch by setting parameter shuffle to True, during initialization.
- Converges after 10^6 training examples, so typically *max_iter* is set to np.ceil(10^6/n)
- When parameter *average* is set to True, the weight vector is updated to the average of weights from previous epochs. When set to an integer, the averaging starts after the set #samples.
- Setting *warm_start* to True, carries forward the weight vector from the previous run, into the current run too.

```
sgd_reg = SGDRegressor(max_iter=1, tol=-np.infty, warm_start=True,
                       penalty=None, learning_rate="constant", eta0=0.0005)

for epoch in range(1000):
    sgd_reg.fit(X_train, y_train)  # continues where it left off
    y_val_predict = sgd_reg.predict(X_val)
    val_error = mean_squared_error(y_val, y_val_predict)
```

- All regression estimators (including `SGDRegressor` and `LinearRegression`) exposes the final set of weights learnt by the model, through attributes *coef_* and *intercept_*
- Finding weight vector can either use normal equation ($\mathbf{w} = \left(\mathbf{X}^T\mathbf{X}\right)^{-1}\mathbf{X}^T\mathbf{y}$), or gradient-descent technique.
- Normal equation method has a complexity of O(m^2) where m is the number of features. This implies that when #features doubles, the calculation could be 4 times as slow.
- Evaluation of all models (including `LinearRegression`) is done using the `score` (or `r2score`) method on a object. It returns the *r2-score*, also called coefficient of determination.

residual sum of squares:

$u = (\mathbf{Xw} - \mathbf{y})^T(\mathbf{Xw} - \mathbf{y})$

Sum of squared error
(actual and predicted label)

$$R^2 = \left(1 - \frac{u}{v}\right)$$

total sum of square
Sum of squared error
(actual and mean predicted $v = (\mathbf{y} - \hat{\mathbf{y}}_{\mathbf{mean}})^T(\mathbf{y} - \hat{\mathbf{y}}_{\mathbf{mean}})$ where, $\hat{y}_{mean} = \frac{1}{n}(\mathbf{Xw})$

- The best possible *r2-score* is 1.0, when the residual sum of squares is 0
- r2-score is 0 for a model that always predicts the same value of y, disregarding the inputs.
- The r2-score can be negative, because the model can be arbitrary worse, and the residual sum can be more than the total sum.
- Following is a list all possible scoring functions. Note that the scoring function are typically negative value of the errors.

Error type	Scoring	Usage
`mean_absolute_error`	`neg_mean_absolute_error`	Common
`mean_squared_error`	`neg_mean_squared_error`	Common
`mean_squared_log_error`	`neg_mean_squared_log_error`	Used when the target has exponential growths like population
`root_mean_squared_error`	`neg_root_mean_squared_error`	Common
`median_absolute_error`	`neg_median_absolute_error`	Used when outliers are present
`r2`	`r2`	-
`max_error`	`max_error`	-

- `max_error` returns maximum error due to training a model.
- In order to avoid any chances of having the **easiest** test-set that yields the least error, always perform cross-validation for robust performance evaluation.
- sklearn implements four cross-validation iterators:
    - `KFold` divides training data into 5 folds, and uses 4 as training and 1 for evaluation.

```
from sklearn.model_selection import cross_val_score
from sklearn.model_selection import KFold
from sklearn.linear_model import linear_regression

lin_reg = linear_regression()
kfold_cv = KFold(n_splits=5, random_state=42)
score = cross_val_score(lin_reg, X, y, cv=kfold_cv)
```

    - `StratifiedKFold` works similar to KFold, with the exception that the folds are made preserving the percentage of samples for each class.
    - `RepeatedKFold` repeats K-Fold n times with different randomization in each repetition.
    - `LeaveOneOut`

```
from sklearn.model_selection import cross_val_score
from sklearn.model_selection import LeaveOneOut
from sklearn.linear_model import linear_regression

lin_reg = linear_regression()
loocv = LeaveOneOut()
score = cross_val_score(lin_reg, X, y, cv=loocv)
```

    - `ShuffleSplit` shuffles the order of data samples in each iteration and then splits it into train and test, and hence robust to class distribution.

```
from sklearn.linear_model import linear_regression
from sklearn.model_selection import cross_val_score
from sklearn.model_selection import ShuffleSplit

lin_reg = linear_regression()
shuffle_split = ShuffleSplit(n_splits=5, test_size=0.2, random_state=42)
score = cross_val_score(lin_reg, X, y, cv=shuffle_split)
```

    - In addition to the existing parameters, `cross_val_score` also accepts *scoring* parameter and can take any of the value in the table discussed under r2-score.
- To obtain test scores for each fold, use `cross_validate`. The results contain *fit_time, score_time, test_score, estimator,* and *train_score*

```
from sklearn.model_selection import cross_validate
from sklearn.model_selection import ShuffleSplit

cv = ShuffleSplit(n_splits=40, test_size=0.3,
                  random_state=0)
cv_results = cross_validate(
    regressor, data, target,
    cv=cv, scoring="neg_mean_absolute_error",
    return_train_score=True,
    return_estimator=True)
```

  NOTE: By default *estimator* and *train_score* are not returned as part of the `cross_validate` output, but only when appropriate parameters are set to True.
- `cross_validate` allows to specify multiple scoring mechanisms unlike `cross_val_score`.

Week4

- In order to use only interaction features in a polynomial transformation, set the parameter *interaction_only* to True like this. This will include only [1,x1, x2, x1x2]. $x1^2$ and $x2^2$ are excluded.

```
1 from sklearn.preprocessing import PolynomialFeatures
2 poly_transform = PolynomialFeatures(degree=2, interaction_only=True)
```

- Ridge Loss = Sum of squared error + regularization_rate * penalty
- Ridge regularization can be performed in two ways. Either using a `Ridge` object, or using `SGDRegressor`object with parameter *penalty* set to 'l2'
- Perform cross-validation on ridge, either using `RidgeCV` object or `GridSearchCV` on `SGDRegressor` object with parameter *penalty* set to 'l2'
- Lasso regularization can be performed in two ways. Either using a `Lasso` object, or using `SGDRegressor`object with parameter *penalty* set to 'l1'
- Perform cross-validation on lasso, either using `LassoCV` object or `GridSearchCV` on `SGDRegressor` object with parameter *penalty* set to 'l1'
- Elasticnet regularization can be performed by using `SGDRegressor`object with parameter *penalty* set to 'elasticnet' and l1_ratio to an appropriate value (<1)
- When *penalty* is set to *'l1'* (lasso), it leads to sparse solutions.
- Penalty α is a non-negative float value. Larger values indicate stronger regularization.