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.

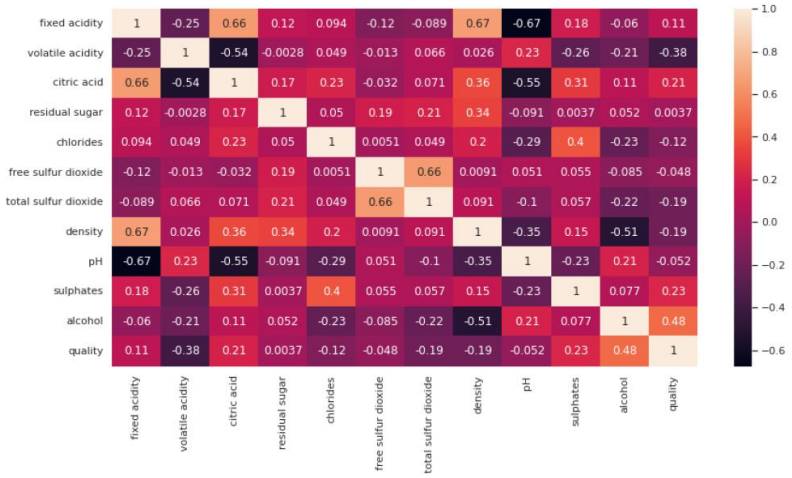
```
from sklearn.model_selection import StratifiedShuffleSplit
split = StratifiedShuffleSplit(n_splits=1, test_size=0.2, random_state=42)
for train_index, test_index in split.split(data, data["quality"]):
  strat_train_set = data.loc[train_index]
  strat_test_set = data.loc[test_index]
```

- 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 `KNNImputer` 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.
  - Scaling techniques should be *learnt* 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.

```
1 from sklearn.pipeline import Pipeline
2 from sklearn.preprocessing import StandardScaler
3 transform_pipeline = Pipeline([
4                               ('imputer', SimpleImputer(strategy="median")),
5                               ('std_scaler', StandardScaler()),])
6 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 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 interval 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 containing 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 specified number 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 $\begin{bmatrix}0\\-1/\sqrt{2}\\-2/\sqrt{2}\\1/\sqrt{2}\\2/\sqrt{2}\end{bmatrix}$
  - `MinMaxScaler` # $\mathbf{x}' = \frac{\mathbf{x} - \mathbf{x}.min}{\mathbf{x}.max - \mathbf{x}.min}$. Example: `MinMaxScaler` Transforms $\begin{bmatrix}15\\2\\5\\-2\\-5\end{bmatrix}$ into $\begin{bmatrix}1\\0.35\\0.5\\0.6\\0\end{bmatrix}$
  - `MaxAbsScaler` # $\mathbf{x}' = \frac{\mathbf{x}}{\text{MaxAbsoluteValue}}$, where $\text{MaxAbsoluteValue} = \max(\mathbf{x}.max, |\mathbf{x}.min|)$
    Note that the resultant values fall within range [-1,1]
    Example: `MaxAbsScaler` transforms $\begin{bmatrix}4\\2\\5\\-2\\-100\end{bmatrix}$ into $\begin{bmatrix}0.04\\0.02\\0.05\\-0.02\\-1\end{bmatrix}$
  - `MinMaxScaler` fits every feature into a range [0, 1]
  - `StandardScaler` is less affected by outliers than `MinMaxScaler`.

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 $\begin{bmatrix}1 & 'male'\\2 & 'female'\\6 & 'female'\\1 & 'male'\\8 & 'male'\\6 & 'female'\end{bmatrix}$ 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: `LabelBinarizer` 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 based 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. It must consist a list of tuples of the form

    (<step_name>, <sklearn_api/`ColumnTransformer` >, <list of the column numbers>).

    Example:
```
estimators = [
  ('simpleImputer', SimpleImputer()),
  ('standardScaler', StandardScaler()),
]
pipe = Pipeline(steps=estimators)
pipe.fit_transform(X)
```

- `FeatureUnion` combines output from several `Pipeline`/`ColumnTransformer` objects by creating a new combined 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, *num_pipeline[-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. It can be used without a pipeline too, directly on the model.

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 statistical property of the training set or a user-specified value.
- `DummyRegressor` makes predictions ignoring the input features, and only based on the y-values passed to the fit() method.

SGDRegressor

- Typically used in a large training setup with greater than 10K samples. For smaller training sets, use `Ridge` or `Lasso`. The advantage of regularized models 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.
- It's not necessary that the loss decreases from one epoch to the next, sometimes it can shoot up before reducing.
- `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 ($\mathbf{w} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$), 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: $u = (\mathbf{X}\mathbf{w} - \mathbf{y})^T(\mathbf{X}\mathbf{w} - \mathbf{y})$ — 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, $\hat{y}_{mean} = \frac{1}{n}(\mathbf{X}\mathbf{w})$

- 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 used during regression. 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.

```
from sklearn.preprocessing import PolynomialFeatures
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. It defaults to 0.0001.
- In the case of *'elasticnet',* effective regularization rate is `(1 - l1_ratio) * l2 + l1_ratio * l1`

Week5

- Classification can be done using either the generic `SGDClassifier`, or one of the following specialized models - `LogisticRegression`, `Perceptron`, `RidgeClassifier`, `LinearSVC`, any of the `sklearn.neighbors` classifiers, or any of the `sklearn.naive_bayes` classifiers.
- The following methods remain same across all classifiers.
    - Model training
        - `fit(X, y[, coef_init, intercept_init, …])`
    - Prediction
        - `predict(X)` predicts class label for samples
        - `decision_function(X)` predicts confidence score for samples
    - Evaluation
        - `score(X, y[, sample_weight])` returns the mean accuracy on the given test data and labels.

RidgeClassifier

- In the case of binary classification, it predicts the class based on the sign of the output, and in the case of multi-class classification, predicts class based on the highest output value. In the former case, it works by minimizing a penalized residual sum of squares $\min_{w} ||\mathbf{X}\mathbf{w} - \mathbf{y}||_2^2 + \alpha||\mathbf{w}||_2^2$
- Regularization rate is specified by using a positive α value during initializing `RidgeClassifier.` Larger values of α imply stronger regularization.
- There exists multiple solver methods for `RidgeClassifier.`
    - Use *sparse_cg* solver for large-scale data.
    - Use *sag/saga* solver if the number of features or samples is large.
    - Use *lsqr* for achieving the fastest solution.
    - Use *auto* to let `RidgeClassifier` automatically select the solver. This is the default.

    NOTE: Faster convergence occurs only when the features are scaled, under all solvers

- If the data is already centered, set parameter *fit_intercept* to False
- `RidgeClassifierCV` implements `RidgeClassifier` with built-in cross validation
- Both `RidgeClassifierCV` implements `RidgeClassifier` can be used with binary/multinomial or even multi-label problems.

Perceptron

- It uses the same underlying implementation as `SGDClassifier` and is typically used for large-scale learning.
- Can be trained in an iterative manner with `partial_fit` method.
- `Perceptron` classifier can be initialized to the weights of the previous run by setting parameter *warm_start* to True.
- Can be used with binary/multinomial classification. It supports multinomial classification by combining multiple binary classifiers using one-vs-all scheme.

LogisticRegression

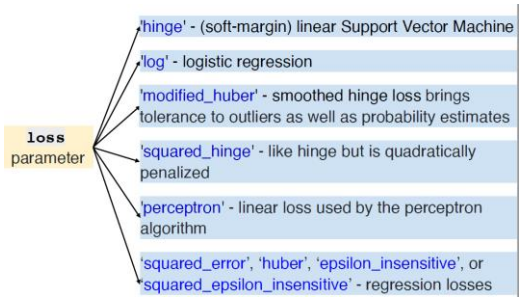
- Works by minimizing (regularization penalty + loss)
  $\arg\min_{\mathbf{w},C}\ \text{regularization penalty}\ + C\ \text{cross entropy loss}$
  NOTE: C is the inverse of the regularization rate λ, and must be positive; larger C implies weaker regularization, and smaller C implies stronger regularization.
- Can be used with binary/ multinomial classification, and one-vs-rest (OVR).
- There exists multiple solver methods for `LogisticRegression`
    - Use *liblinear* for smaller datasets.
    - Use *sag/saga* for larger datasets.
    - Use *liblinear, lbfgs, newton-cg* for unscaled datasets.
    - *liblinear* can handle only OVR, and not multinomial problems.
    - *Lbfsg* is the default solver.
- By default, uses *'l2'* penalty ,but can be changed to one of *'l1', 'l2', 'elasticnet'* or *'none'*
- Following table shows support for penalties by different solvers.

Solver	Penalty
'newton-cg'	['l2', 'none']
'lbfgs'	['l2', 'none']
'liblinear'	['l1', 'l2']
'sag'	['l2', 'none']
'saga'	['elasticnet', 'l1', 'l2', 'none']

- Use parameter *class_weight* to handle class-imbalance in the dataset, where mistakes in a class can be penalized. Higher values of *class_weight* will put more emphasis on the corresponding class.
- `LogisticRegressionCV` implements logistic regression with in built cross validation support to find the best values of parameters *C* and *l1_ratio* according to the specified *scoring* attribute.
- `LogisticRegressionCV` can also be used with binary/ multinomial classification, and one-vs-rest (OVR).

SGDClassifier

- Uses gradient descent for optimization, where gradient loss is estimated for each sample at a time, and weights updated with a decreasing learning schedule.
- Provides greater control on the optimization process through its hyperparameters
  - *loss* (see below)
  - *penalty* (l1, l2, elasticnet). Default is *elasticnet*.
  - *learning_rate* (constant, optimal, invscaling, adaptive). Default is *invscaling*.
  - *early_stopping* (True, False)
- Parameter *loss* can be one of



- By default, `SGDClassifier` uses *hinge loss* and hence trains linear SVM classifier.
- For most part, `SGDClassifier` works very similar to `SGDRegressor`, including the use of parameters and their default values.
- Used with binary/multinomial classification, and one-vs-rest (OVR). It supports multinomial classification by combining multiple binary classifiers using one-vs-all scheme.
- Supports large datasets, more than 10^5 examples and 10^5 features.
- Widely used in text classification and natural language processing.
- Advantages include efficiency and ease of implementation, but disadvantageous because it requires a lot of hyperparameters, is highly sensitive to feature scaling. It also requires shuffling of data before fitting the model in each iteration.
- `SGDClassifier(loss='log')` is equivalent to `LogisticRegression(solver='sgd')`
- `SGDClassifier(loss='perceptron')` is equivalent to `Perceptron()`
- `SGDClassifier(loss='hinge')` is equivalent to `LinearSVC()`

- `SGDClassifier(loss='squared_error')` is equivalent to `a least-square classifier.`

- Use `type_of_target` to check if the label input is *binary, multi-class, continuous, multilabel-indicator or multiclass-multioutput.*
- If the labels are represented in a matrix form,
    - If the number of classes are two, it's multilabel-indicator (Ex. [[-1,1],[1,-1]])
    - If there are more than two classes, it's multiclass-multioutput. (Ex. [[0,1,2],[0,1,2]])
- If the labels are represented in a vector form,
    - if the number of classes are two, it's binary (Ex. [0,1])
    - If there are more than two classes, it's multi-class. (Ex. [0,1,2])
    - If the values belong to a continuous range (like a decimal), it's continuous. (Ex. [1, 2.1, 3.4])
- All `sklearn` classifiers can be used with used with multiclass classification by default, Use `sklearn.multiclass` module only when you want to experiment with different multiclass strategies.
- `sklearn` implements the following multiclass strategies
    - `OneVsRestClassifier (OVR)` fits one classifier per class, is computationally very efficient and requires only k classifiers, one for each class.
    - `OneVsOneClassifier (OVA)` fits one classifier per pairs of classes, where it predicts the class with maximum votes. A tie among classes is broken by selecting the class with the highest aggregate classification confidence.
    - Both strategies above support multilabel classification, if you provide labels as (n, k) indicator matrix.
- `sklearn` implements the following multilabel/multioutput strategies
    - `MultiOutputClassifier` fits one classifier per target.
    - `Classifier` fits binary classifiers in a chain, so that output of one classifier can be combined with other such classifiers in the chain, to make a multilabel model.
- Following is a list all possible scoring functions used during classification - accuracy_score, balanced_accuracy_score, top_k_accuracy_score, roc_auc_score, precision_score, recall_score, f1_score
- In the case of multilabel classification , `confusion`_matrix returns a matrix and is interpreted differently than in the case of regression. Entry (*i, j*) is the number of observations in class *i*, but predicted to be in class *j*
- Confusion matrix can be displayed with `ConfusionMatrixDisplay` API in `sklearn.metrics`, from any of
    - Confusion matrix
      ```
      1 ConfusionMatrixDisplay(confusion_matrix=cm, display_labels=clf.classes_)
      ```
      Estimator
      ```
      1 ConfusionMatrixDisplay.from_estimator(clf, X_test, y_test)
      ```
    - Predictions
      ```
      1 ConfusionMatrixDisplay.from_predictions(y_test, y_pred)
      ```

- In order to use binary metrics in multi-class/multi-label problems, use one the following average parameters - macro, weighted, micro, samples or None.

Week6

- Naive Bayes classifier applies Bayes' theorem with the "naive" assumption of conditional independence between every pair of features given the value of the class variable. This can be mathematically represented as $P(x_i|y, x_1, ..., x_{i-1}, x_{i+1}, ..., x_m) = P(x_i|y)$
- Algos implemented in the `sklearn.naive_bayes` models are `GaussianNB`, `BernoulliNB`, `MultinomialNB`, `CategoricalNB`, `ComplementNB`
- Building an `SGDClassifier`
  1. **Training data**: (features, label) or $(\mathbf{X}, y)$, where label y is a **discrete** number from a finite set.**Features** in this case are pixel values of an image.
  2. **Model :**

$$z = w_0x_0 + w_1x_1 + w_2x_2 + \ldots + w_mx_m$$
$$= \mathbf{w}^T\mathbf{x}$$

  and passing it through the sigmoid non-linear function (or Logistic function)

$$\sigma(z) = \frac{1}{1 + e^{-z}} = \frac{1}{1 + exp(-z)}$$

  3. **Loss function:**

$$J(\mathbf{w}) = -\frac{1}{n}\sum \left[y^{(i)}log(h_\mathbf{w}(\mathbf{x}^{(i)})) + (1 - y^{(i)})(1 - log(h_\mathbf{w}(\mathbf{x}^{(i)})))\right]$$

  4. **Optimization:**
     Gradient Descent
- In the case of `Perceptron` and `RidgeClassifier`, while dealing with binary classification problems, the classes should be -1 and 1. However, in the case of `DummyClassifier` or `SGDClassifier`, the classes should 0 and 1.