# Machine Learning with Python – SciKit-learn Part 2

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## Logistic regression

- Limitations of perceptron
  - Easy introduction to machine learning for classification, but
  - Won't converge if categories not perfectly linearly separable
    - E.g. weights could be updated indefinitely if even one misclassification
  - Another alternative: Logistic Regression
- Logistic regression
  - Classification technique
  - Works well for linearly separable categories
  - One of most widely used classification algorithms in industry
  - Linear model for binary classification (like Perceptron)
  - Can also be used for multi-class classification

## Logistic regression

- Probability of event we want to predict: p
- Odds ratio: p/(1-p)
- Logit(p) =  $\log(p/(1-p))$  inverse of logit function is the logistic

function  $\phi(z)$ 

$$\phi(z) = p$$
: probability of our event of interest where  $z = \mathbf{w}^T$ .  $\mathbf{x} = \mathbf{logit}(\mathbf{p}) = \mathbf{log} \frac{\mathbf{p}}{1 - \mathbf{p}}$ 

where 
$$m{w} = \begin{bmatrix} w_1 \\ \cdots \\ w_m \end{bmatrix}$$
 ,  $m{x} = \begin{bmatrix} x_1 \\ \cdots \\ x_m \end{bmatrix}$ 

$$z = log rac{p}{1-p}$$
Implies
$$p = rac{1}{1+e^{-z}}$$
i.e.
$$\phi(z) = rac{1}{1+e^{-z}}$$

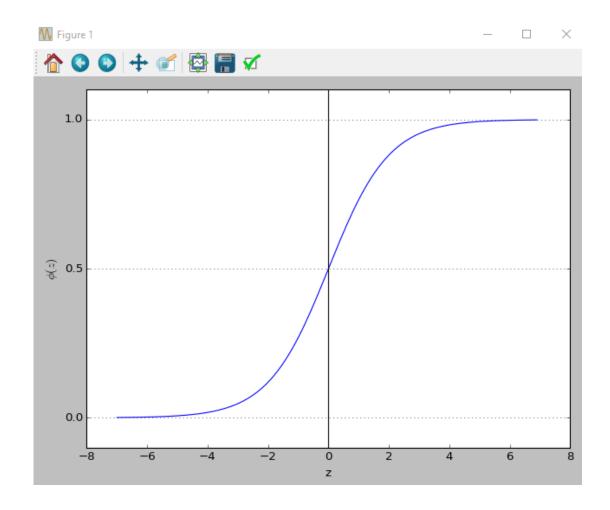
As 
$$z \to \infty$$
,  $\phi(z) \to 1$ 

As  $z \to -\infty$ ,  $\phi(z) \to 0$ 

$$\phi(z) = P(y = 1 | x; w)$$

## What does the sigmoid curve look like?

```
[29]: import matplotlib.pyplot as plt
...: import numpy as np
     def sigmoid(z):
        return 1.0 / (1.0 + np.exp(-z))
...: z = np.arange(-7, 7, 0.1)
    phi_z = sigmoid(z)
    plt.plot(z, phi_z)
...: plt.axvline(0.0, color='k')
    plt.ylim(-0.1, 1.1)
...: plt.xlabel('z')
...: plt.ylabel('$\phi (z)$')
...: # y axis ticks and gridline
    plt.yticks([0.0, 0.5, 1.0])
    ax = plt.gca()
    ax.yaxis.grid(True)
     plt.tight_layout()
    # plt.savefig('./figures/sigmoid.png', dpi=300)
    plt.show()
```



## Logistic regression

Predicted probability converted to binary outcome via unit step function:

$$\hat{y} = \begin{cases} 1 & if \phi(z) \ge 0.5 \\ 0 & otherwise \end{cases}$$

Equivalently:

$$\hat{y} = \begin{cases} 1 & \text{if } z \ge 0.0 \\ 0 & \text{otherwise} \end{cases}$$

## Applications of logistic regression

- Weather forecasting e.g. probability of rain
- Marketing/Sales: Likelihood of a customer purchasing a product
- HR/Management: Likelihood of an employee leaving or joining a firm
- Accounting: Likelihood of an accounting transaction being fraudulent
- Manufacturing/operations: Likeliood of a part being defective
- IT: Likelihood of a web log entry being a hacking attempt

# Ingesting and preparing data (repeated)

```
[4]: from sklearn import datasets
  ...: import numpy as np
  ...: iris = datasets.load iris()
  ...: X = iris.data[:, [2, 3]]
  ...: y = iris.target
  ...: print('Class labels:', np.unique(y))
lass labels: [0 1 2]
In [5]: from sklearn.model selection import train test split
  ...: X_train, X_test, y_train, y_test = train test split(
  ...: X, y, test_size=0.3, random_state=0)
 [6]: from sklearn.preprocessing import StandardScaler
  ...: sc = StandardScaler()
  ...: sc.fit(X train)
  ...: X train std = sc.transform(X train)
  ...: X_test_std = sc.transform(X_test)
```

## Perform logistic regression

- 1. Import logistic regression class from scikit-learn
- 2. Create an object Ir of the logistic regression class
  - "C" is a parameter that controls for overfitting lower
     C implies less overfitting
- 3. Fit the model on the training dataset

## Predict using learned model

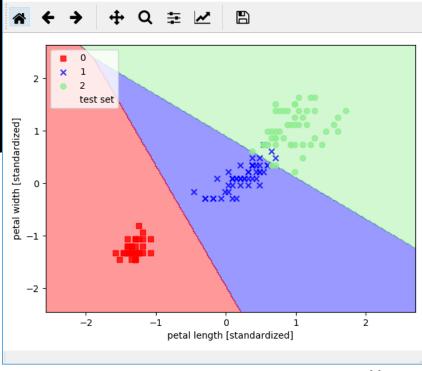
```
In [10]: y_pred = lr.predict(X_test_std)
In [11]: from sklearn.metrics import accuracy_score
    ...:
    ...: print('Accuracy: %.2f' % accuracy_score(y_test, y_pred))
    ...:
Accuracy: 0.98
```

#### Predicting individual test sample:

i.e. change of 93.7 percent that sample belongs to Iris-Virginica class, Chance of 6.3 percent that saple is Iris-Versicolor

```
[19]: b = lr.predict_proba(X_test_std[1, :].reshape(1, -1))
 [20]: np.around(b,decimals=3)
 [20]: array([[ 0.001, 0.999, 0. ]])
  [21]: c = lr.predict_proba(X_test_std[2, :].reshape(1, -1))
 [22]: np.around(c,decimals=3)
 t[22]: array([[ 0.817, 0.183, 0. ]])
  [23]: d = lr.predict_proba(X_test_std[3, :].reshape(1, -1))
[n [24]: np.around(d,decimals=3)
       array([[ 0. , 0.414, 0.586]])
```

## Plot the points



## Precision, recall, f1-score

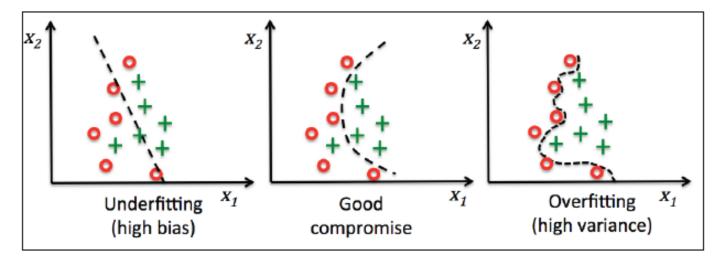
```
In [16]: from sklearn.metrics import classification_report, confusion_matrix
   ...: print(confusion_matrix(y_test,y_pred))
   ...: print(classification_report(y_test,y_pred))
  0 0 11]]
            precision
                         recall f1-score
                                            support
                 1.00
                           1.00
                                     1.00
                                                 16
                 1.00
                           0.94
                                     0.97
                                                 18
                 0.92
                                                 11
                           1.00
                                     0.96
avg / total
                           0.98
                                     0.98
                                                 45
                 0.98
```

## Overfitting:

- Model performs well on training data
- But not on test data
- Also, we can say model has "high variance"
- When model is too complex given underlying data

## • Underfitting:

- Not complex enough to capture training data pattern well
- Therefore, low performance on unseen data



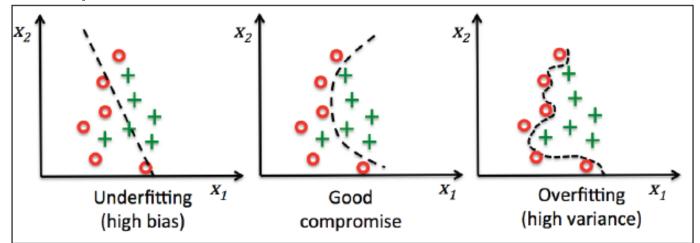
## Variance vs Bias

### • Variance:

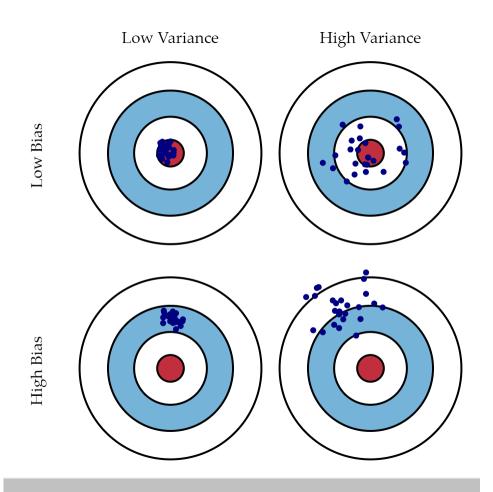
- Measures variability of model predictions if we retrained model on different subsets of training dataset
- If variance is high, model is sensitive to randomness in training data

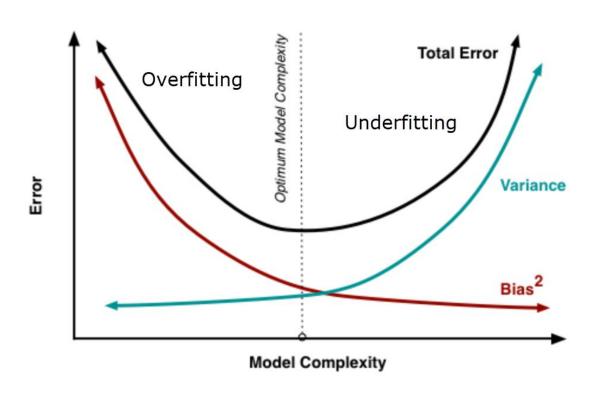
### Bias

- Measures how far off predictions are from correct values if model is rebuilt multiple times on different training sets
- Measure of systematic error not due to randomness



## Bias and variance





## Regularization

- Tune the model complexity via regularization
- Helps find a good bias-variance tradeoff
- Helps to handle
  - high correlation among features (high collinearity)
  - Filter noise from data
  - Prevent overfitting
- Idea:
  - Introduce additional information (bias) penalize extreme parameter weights
- Most common: L2 regularization (also known as L2 shrinkage or L2 weight decay)

$$\frac{\lambda}{2} \|\mathbf{w}\|^2 = \frac{\lambda}{2} \sum_{j=1}^m w_j^2$$

## Regularization

Add regularization term to cost function used to change weights:

$$J(w) = \left[ \sum_{i=1}^{n} \left( -\log \left( \phi(z^{(i)}) \right) + \left( 1 - y^{(i)} \right) \left( -\log \left( 1 - \phi(z) \right) \right) \right) \right] + \frac{\lambda}{2} ||w||^{2}$$

Parameter "C" in Logistic Regression method:

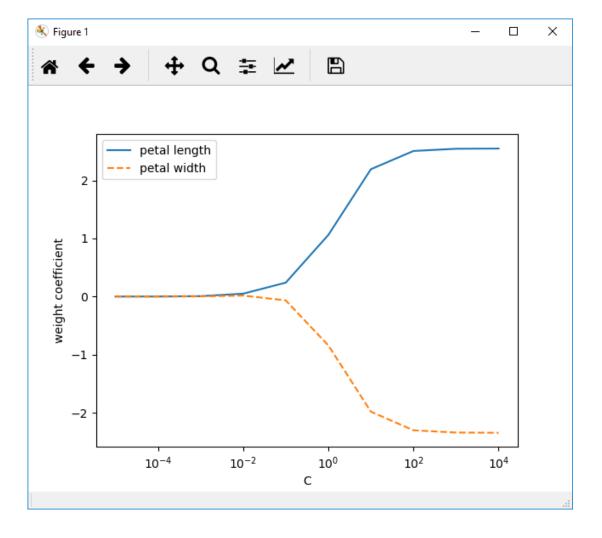
$$C = \frac{1}{\lambda}$$

Lower the C, higher the regularization strength – and lesser the overfitting (but more underfitting)

```
In [12]: weights, params = [], []
  ...: for c in np.arange(-5., 5.):
  ...: lr = LogisticRegression(C=10.**c, random_state=0)
  ...: lr.fit(X_train_std, y_train)
  ...: y_pred = lr.predict(X_test_std)
  ...: print('Accuracy: %.2f' % accuracy_score(y_test, y_pred))
Accuracy: 0.60
Accuracy: 0.60
Accuracy: 0.60
Accuracy: 0.60
Accuracy: 0.60
Accuracy: 0.80
Accuracy: 0.96
Accuracy: 0.98
Accuracy: 0.98
Accuracy: 0.98
```

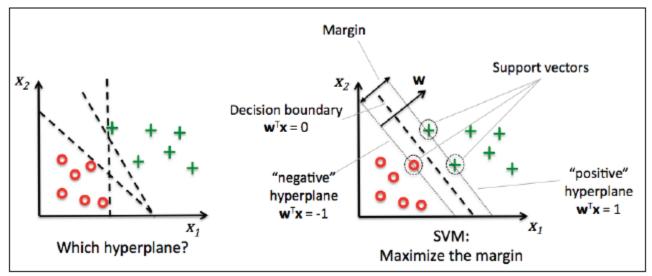
```
[n [25]: weights, params = [], []
  ...: for c in np.arange(-5., 5.):
   ...: lr = LogisticRegression(C=10.**c, random_state=0)
  ...: lr.fit(X_train_std, y_train)
   ...: weights.append(lr.coef_[1])
  ...: params.append(10**c)
   ...: weights = np.array(weights)
   ...: plt.plot(params, weights[:, 0],
   ...: label='petal length')
   ...: plt.plot(params, weights[:, 1], linestyle='--',
   ...: label='petal width')
   ...: plt.ylabel('weight coefficient')
   ...: plt.xlabel('C')
   ...: plt.legend(loc='upper left')
   ...: plt.xscale('log')
   ...: # plt.savefig('./figures/regression_path.png', dpi=300)
   ...: plt.show()
```

As we decrease C, i.e.
 increase regularization
 strength (lambda), the
 weight coefficients shrink –
 their absolute value
 decreases (i.e. less
 overfitting)

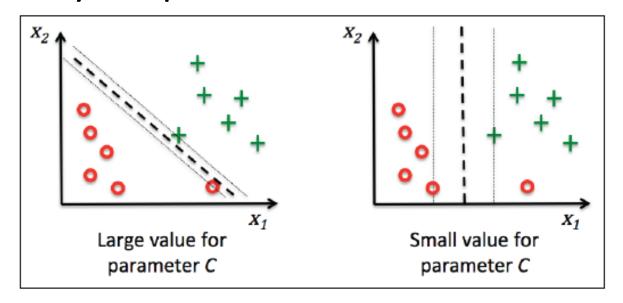


## Support Vector Machines (SVM)

- Extension of perceptron
- In perceptron, minimize misclassification error
- SVM: optimization objective is to maximize the margin
  - Distance between decision boundary ("separating hyperplane") and training samples closest to this hyperplane (the "support vectors")



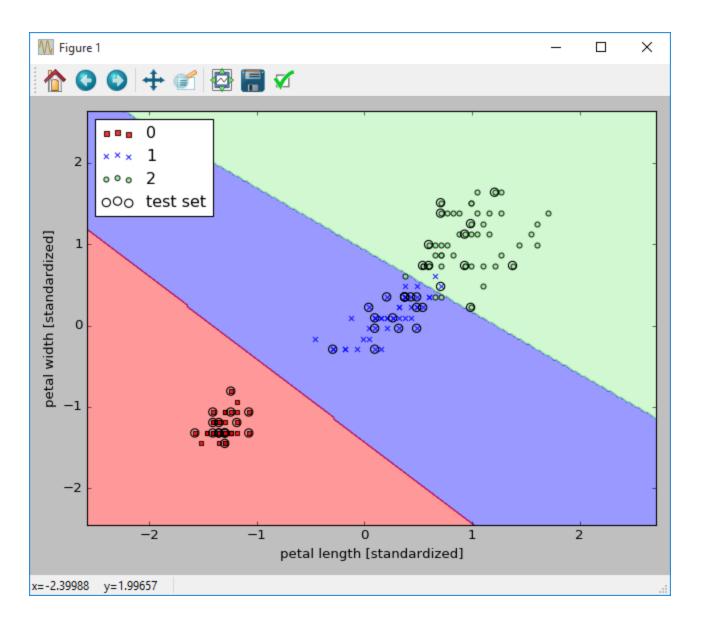
## Non-linearly separable case — slack variables



- ➤ Variable "C" control penalty for misclassification
- ➤ Large "C" large error penalties for misclassification
- > Small "C" small error penalties for misclassification when we are less strict about misclassification errors
- > Decreasing "C" (inverse of regularization constant) increases bias and lowers variance of model

$$C = \frac{1}{\lambda}$$

```
In [37]: from sklearn.svm import SVC
...:
...: svm = SVC(kernel='linear', C=1.0, random_state=0)
...: svm.fit(X_train_std, y_train)
...:
...: plot_decision_regions(X_combined_std, y_combined,
...: classifier=svm, test_idx=range(105, 150))
...: plt.xlabel('petal length [standardized]')
...: plt.ylabel('petal width [standardized]')
...: plt.legend(loc='upper left')
...: plt.tight_layout()
...: # plt.savefig('./figures/support_vector_machine_linear.png', dpi=300)
...: plt.show()
```



```
[11]: y_pred = svm.predict(X_test_std)
  [13]: from sklearn.metrics import accuracy score
   ...: print('Accuracy: %.2f' % accuracy_score(y_test, y_pred))
Accuracy: 0.98
  [12]: from sklearn.metrics import classification_report, confusion_matrix
   ...: print(confusion_matrix(y_test,y_pred))
   ...: print(classification_report(y_test,y_pred))
[16 0
 0 17 1]
 0 0 11]]
            precision
                         recall f1-score
                                            support
                 1.00
                          1.00
                                     1.00
                                                 16
                 1.00
                           0.94
                                     0.97
                                                 18
                 0.92
                           1.00
                                     0.96
                                                 11
   / total
                 0.98
                           0.98
                                     0.98
                                                 45
```

## Logistic regression vs. SVM

- Linear logistic regression (LR) and linear SVM similar results
- LR more prone to outliers than SVM
- SVM mostly cares about points closest to decision boundary (support vectors)
- LR is simpler model, implemented more easily
- LR is more easily updated advantage with streaming data

# Data Preprocessing

```
import pandas as pd
from io import StringIO

# Creating a sample csv data and
# |dataframe with null values
csv_data = '''A,B,C,D
1.0,2.0,3.0,4.0
5.0,6.0,,8.0
0.0,11.0,12.0,'''
df = pd.read_csv(StringIO(csv_data))
df
```

```
In [6]: df
Out[6]:

A B C D
0 1.0 2.0 3.0 4.0
1 5.0 6.0 NaN 8.0
2 0.0 11.0 12.0 NaN
```

```
In [7]: df.isnull().sum()
Out[7]:
A      0
B      0
C      1
D      1
dtype: int64
```

```
In [9]: df
Out[9]:
          A     B     C     D
0 1.0     2.0     3.0     4.0
1 5.0     6.0     NaN     8.0
2 0.0     11.0     12.0     NaN

In [10]: df.dropna()
Out[10]:
          A     B     C     D
0 1.0     2.0     3.0     4.0
```

```
In [12]: df.dropna(axis=1)
Out[12]:

A B
0 1.0 2.0
1 5.0 6.0
2 0.0 11.0
```

```
In [13]: df.dropna(how='all')
Out[13]:

A B C D
0 1.0 2.0 3.0 4.0
1 5.0 6.0 NaN 8.0
2 0.0 11.0 12.0 NaN
```

```
[14]: df.dropna(thresh=4)
         С
              D
[15]: df.dropna(thresh=3)
                D
1.0
     2.0
           3.0
               4.0
5.0
     6.0
           NaN
               8.0
    11.0 12.0 NaN
0.0
[16]: df.dropna(subset=['C'])
                 D
1.0
     2.0
           3.0 4.0
0.0
    11.0
          12.0 NaN
```

```
# Handling categorical data

df = pd.DataFrame([
  ['green ','M',10.1,'class1'],
  ['red','L',13.5,'class2'],
  ['blue','XL',15.3,'class1']])

df.columns = ['color','size','price','classlabel']

df
```

```
# Mapping ordinal features
size_mapping = {
'XL': 3,
'L': 2,
'M': 1}
df['size'] = df['size'].map(size_mapping)
df
```

```
In [40]: df
Out[40]:
    color size price classlabel
0 green    1    10.1    class1
1    red    2    13.5    class2
2    blue    3    15.3    class1
```

```
# Reverting to the original categorical variables
inv_size_mapping = {v: k for k, v in size_mapping.items()}
df['size'] = df['size'].map(inv_size_mapping)
df
```

```
In [42]: df
Out[42]:
    color size price classlabel
0 green    M   10.1     class1
1    red    L   13.5     class2
2    blue    XL   15.3     class1
```

```
# Automatically replace (nominal)
# |class-labels with numbers
class_mapping = {
    label:idx for idx,label in
    enumerate(np.unique(df['classlabel']))}
```

```
In [45]: class_mapping
Out[45]: {'class1': 0, 'class2': 1}
```

```
[47]: df
  color size price classlabel
 green M 10.1 class1
          L 13.5 class2
    red
   blue XL 15.3 class1
[n [48]: df['classlabel'] = df['classlabel'].map(class_mapping)
n [49]: df
  color size price classlabel
          M 10.1
 green
    red L 13.5
   blue XL 15.3
```

```
# Get back the original class labels
inv_class_mapping = {v: k for k, v in class_mapping.items()}
df['classlabel'] = df['classlabel'].map(inv_class_mapping)
```

```
# Alternately, use | scikitlearn module
# to perform encoding
from sklearn.preprocessing import LabelEncoder
class_le = LabelEncoder()
y = class_le.fit_transform(df['classlabel'].values)
y
In [56]: v
```

array([0, 1, 0], dtype=int64)

```
In [57]: class_le.inverse_transform(y)
Out[57]: array(['class1', 'class2', 'class1'], dtype=object)
```

### One-hot encoding

Problem with the following approach: order implied by number

```
# Handling categorical data

df = pd.DataFrame([
   ['green ','M',10.1,'class1'],
   ['red','L',13.5,'class2'],
   ['blue','XL',15.3,'class1']])

df.columns = ['color','size','price','classlabel']

df
```

```
# Mapping ordinal features
size_mapping = {
'XL': 3,
'L': 2,
'M': 1}
df['size'] = df['size'].map(size_mapping)
df
```

```
In [40]: df
Out[40]:
    color size price classlabel
0 green    1    10.1    class1
1    red    2    13.5    class2
2    blue    3    15.3    class1
```

#### One-hot encoding

```
In [40]: pd.get_dummies(df[['price', 'color', 'size']])
Out[40]:
    price size color_blue color_green color_red
0 10.1 1 0 1 0
1 13.5 2 0 0 1
2 15.3 3 1 0 0
```

# Partitioning a dataset into training and test sets

- Test set: the ultimate test of our model before we use it in the real world
- Import data

## Train-test-split

## Feature scaling

- When to consider feature scaling
  - Logistic regression, SVM, perceptrons, neural networks.
  - K-nearest neighbors with a Euclidean distance measure with features contributing equally
  - K-means, Linear discriminant analysis, principal component analysis, kernel principal component analysis.
  - Decision trees, random forests no need to worry about feature scaling
- Two types of feature scaling
  - Normalization
  - Standardization

#### Normalization

• Normalization: bring features to [0,1] range:

$$x_{norm}^{(i)} = \frac{x^{(i)} - x_{\min}}{x_{\max} - x_{\min}}$$

from sklearn.preprocessing import MinMaxScaler
mms = MinMaxScaler()
X\_train\_norm = mms.fit\_transform(X\_train)
X\_test\_norm = mms.transform(X\_test)

Sensitive to outliers

#### Standardization

 Many linear models (e.g. Logistic Regression, SVM) initialize weights to 0 or small random values close to 0

• Sometimes standardization (mean 0, std dev 1) helps learn weights

better:

 $x_{std}^{(i)} = \frac{x^{(i)} - \mu_x}{\sigma_x}$ 

```
from sklearn.preprocessing import StandardScaler

stdsc = StandardScaler()
X_train_std = stdsc.fit_transform(X_train)
X_test_std = stdsc.transform(X_test)
```

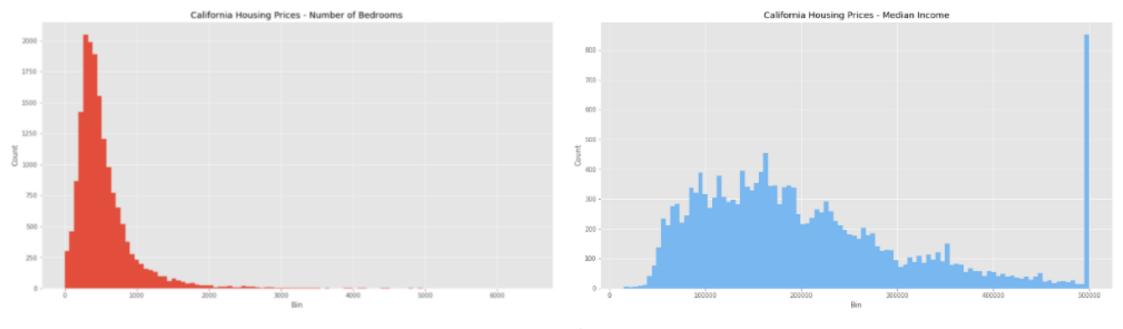
- Standardization preserves useful information about outliers
- Algorithm less sensitive to outliers than in min-max scaling

### When to use what method

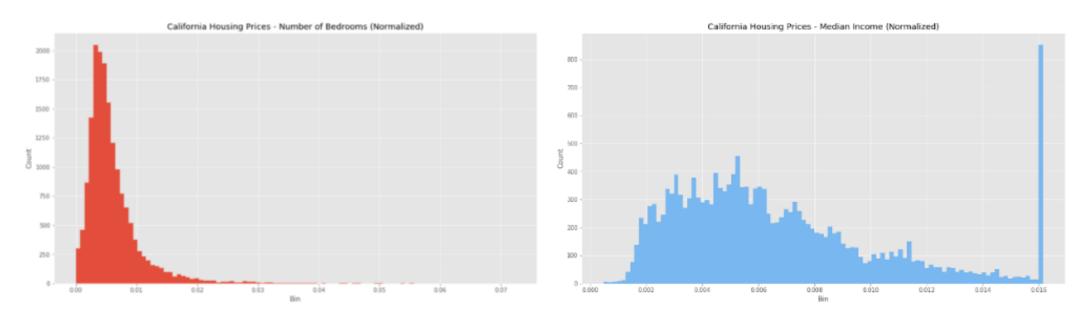
- Normalize when
  - distribution of data is unknown
  - distribution is known to be not Gaussian (i.e. bell curve)
  - outliers are not a concern
  - standard deviation very small
  - algorithm does not make assumptions about the distribution of data (e.g. k-nearest neighbors and artificial neural networks)
- Standardize otherwise

#### Normalization vs Standardization

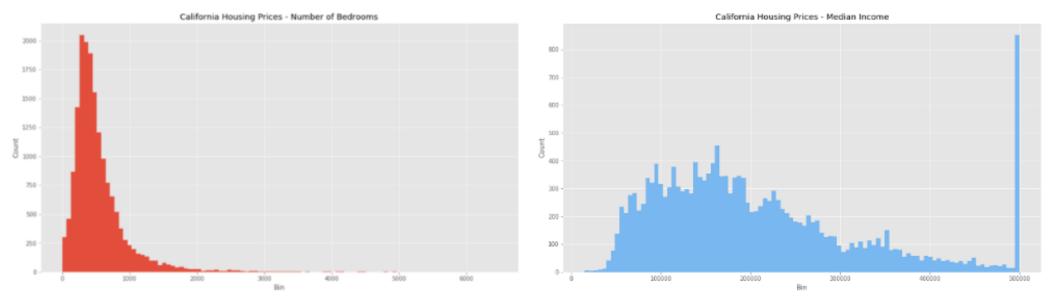
- Normalize
  - useful for optimization algorithms e.g. gradient descent that weight inputs (e.g. artificial neural networks).
  - also for algorithms that use distance measurements e.g. K-Nearest-Neighbors (KNN).
- Standardize (subtract from mean, divide by std dev)
  - linear regression, logistic regression, SVM and linear discriminant analysis
- When in doubt, do both and see which works better



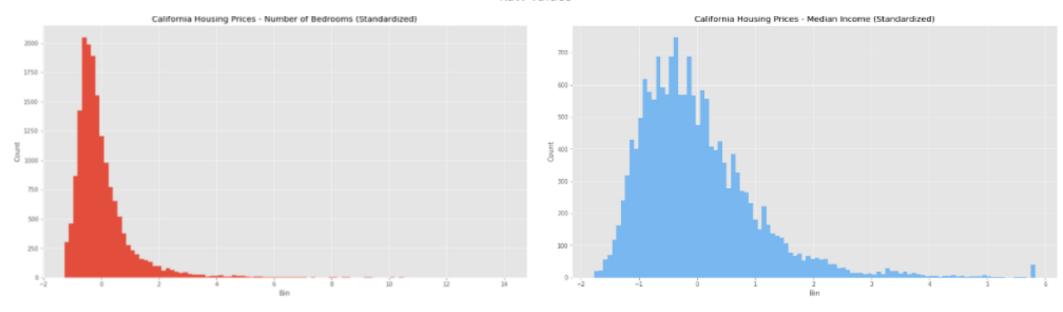
#### Raw Values



Normalized Values 16



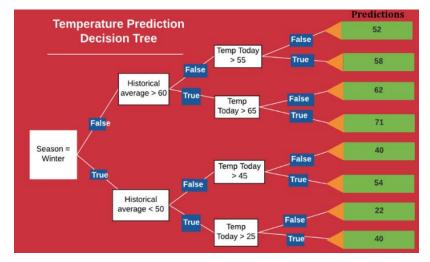




Standardized Values

### Random forest – brief overview

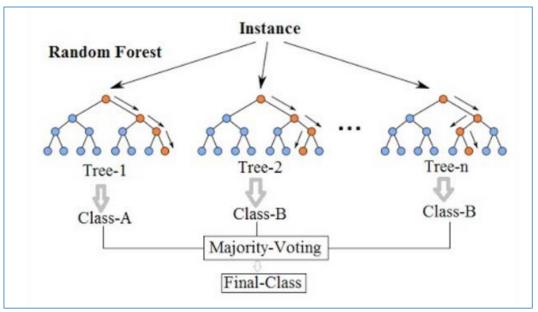
One decision tree:



 Random forest: many decision trees – on random subsets of training data – on random features – averaged

#### Source:

https://medium.com/@williamkoehrsen/random-forest-simple-explanation-377895a60d2d



# Assessing feature importance with Random Forests

- Import the random forest classifier
- Create the model, with hyper-parameters
   "n\_estimators": number of trees
- 3. Fit the model on your data
- 4. Extract feature-importances
- 5. Sort feature-importances

# Assessing feature importance with Random Forests

6. Print all features in descending order of importance

```
for f in range(X_train.shape[1]):
         print("%2d) %-*s %f" % (f + 1, 30,
                                  feat_labels[indices[f]],
                                  importances[indices[f]])
Color intensity
                                0.182483
Proline
                                0.158610
Flavanoids
                                0.150948
OD280/OD315 of diluted wines
                               0.131987
Alcohol
                                0.106589
                                0.078243
Total phenols
                                0.060718
Alcalinity of ash
                                0.032033
Malic acid
                                0.025400
Proanthocyanins
                                0.022351
Magnesium
                                0.022078
Nonflavanoid phenols
                                0.014645
Ash
                                0.013916
```