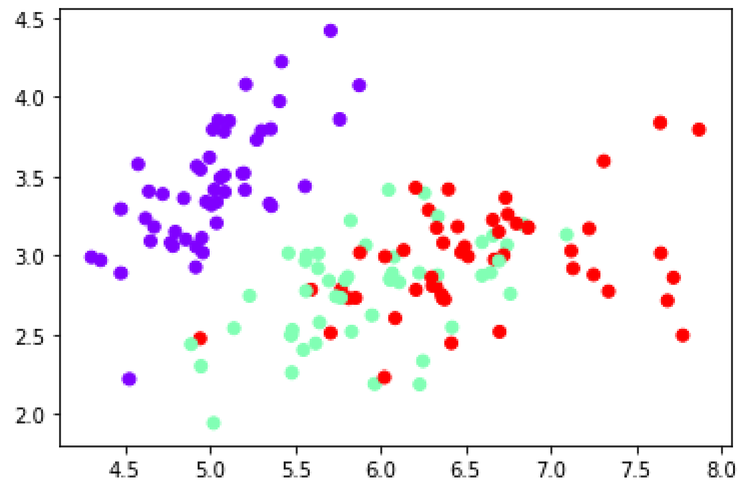
In [1]:
```python
import numpy as np
import scipy.stats
import matplotlib.pyplot as plt
%matplotlib inline
from sklearn import neighbors, datasets
from sklearn.metrics import pairwise_distances
from sklearn.utils import shuffle

# import some data to play with
iris = datasets.load_iris()
X = iris.data[:, :2]   # we only take the first two features
X = X + 0.05 * np.random.RandomState(0).randn(*X.shape) # Add random noi
se since iris has exact values
y = iris.target
X, y = shuffle(X, y, random_state=0)
plt.scatter(X[:, 0], X[:, 1], c=y, cmap='rainbow')
print(X.shape)
```

```
(150, 2)
```



```
In [2]: class SimpleKNNClassifier():
            def __init__(self, X_train, y_train, k=1):
                self.X_train = X_train
                self.y_train = y_train
                self.k = k

            def predict(self, X):
                # Compute distances
                D = np.nan * np.ones((X.shape[0], self.X_train.shape[0]))
                for i, x in enumerate(X):
                    for j, xt in enumerate(self.X_train):
                        D[i, j] = np.linalg.norm(x-xt)
                # Much faster vectorized version using sklearn's pairwise distan
        ces function
                D2 = pairwise_distances(X, self.X_train, metric='euclidean')
                assert np.allclose(D, D2), 'Should be the same'

                # Get the indices of the top k smallest distances
                sorted_idx = np.argsort(D, axis=1)

                # For each data point get mode
                y = np.array([
                    scipy.stats.mode(self.y_train[sidx[:self.k]])[0][0]
                    for sidx in sorted_idx
                ])
                # Faster vectorized version
                y_ind = self.y_train[sorted_idx[:,:self.k]]
                y2 = scipy.stats.mode(y_ind, axis=1)[0].ravel()
                assert np.all(y == y2), 'Should be the same'
                return y

        k = 1 #3 or 10
        knn = SimpleKNNClassifier(X, y, k=k)
        y_pred = knn.predict(X)
        accuracy = np.mean(y == y_pred)
        print(f'The accuracy on the training data for k={k} is: {accuracy*100:.1
        f}%')
```

```
The accuracy on the training data for k=1 is: 100.0%
```

## This seems odd, do we really think our method has PERFECT accuracy?

## Suppose we only had 100 points for training and then received 50 new flower measurments

In [3]:
```python
# Use first 100 points
X_train = X[:100,:]
y_train = y[:100]

# Setup model
for k in [1, 3, 5, 7, 9, 12]:
    knn = SimpleKNNClassifier(X_train, y_train, k=k)

    # Predict on training data
    y_pred = knn.predict(X_train)
    accuracy = np.mean(y_train == y_pred)
    print(f'The accuracy on the training data for k={k} is: {accuracy*10
0:.1f}%')

    # Now let's test our method on the new flowers
    X_new = X[100:,:]
    y_new = y[100:]
    y_pred = knn.predict(X_new)
    accuracy = np.mean(y_new == y_pred)
    print(f'The accuracy on the new data for k={k} is: {accuracy*100:.1
f}%\n')
```

```
The accuracy on the training data for k=1 is: 100.0%
The accuracy on the new data for k=1 is: 72.0%

The accuracy on the training data for k=3 is: 83.0%
The accuracy on the new data for k=3 is: 74.0%

The accuracy on the training data for k=5 is: 83.0%
The accuracy on the new data for k=5 is: 78.0%

The accuracy on the training data for k=7 is: 82.0%
The accuracy on the new data for k=7 is: 80.0%

The accuracy on the training data for k=9 is: 82.0%
The accuracy on the new data for k=9 is: 82.0%

The accuracy on the training data for k=12 is: 83.0%
The accuracy on the new data for k=12 is: 82.0%
```

## The above generalization accuracy estimation algorithm is known as using a train/test split

## Cross validation is a better estimate of generalization accuracy

In [4]:
```
def cv_estimate(X, k, n_splits=3):
    # Setup split indices
    split_ind = np.floor(np.linspace(0, X.shape[0], num=n_splits+1))
    # Loop over splits
    accuracy_list = []
    for split_start, split_end in zip(split_ind[:-1], split_ind[1:]):
        # Setup boolean array to select test set
        test = np.zeros(X.shape[0], dtype=bool)  # Initialize false bool
ean array
        test[int(split_start):int(split_end)] = True  # Set test element
s to true

        # Create train and test sets
        X_train = X[~test, :] # ~ is used to denote "not" for all boolea
n values
        y_train = y[~test]
        X_test = X[test, :]
        y_test = y[test]

        # Train model for this split using X_train and y_train
        knn = SimpleKNNClassifier(X_train, y_train, k=k)

        # Compute accuracy on test split
        y_pred = knn.predict(X_test)
        accuracy = np.mean(y_test == y_pred)
        accuracy_list.append(accuracy)
    # Take mean of accuracy
    return np.mean(accuracy_list)

for k in [1, 3, 5, 7, 9, 12]:
    # n_splits is often 3, 5, 10; X.shape[0] (i.e., one split per sampl
e) is known as Leave One Out (LOO)
    cv_acc = cv_estimate(X, k, n_splits=3)
    print(f'CV accuracy estimate for k={k} is {100*cv_acc:.1f}%')
```

```
CV accuracy estimate for k=1 is 74.7%
CV accuracy estimate for k=3 is 76.0%
CV accuracy estimate for k=5 is 76.7%
CV accuracy estimate for k=7 is 78.0%
CV accuracy estimate for k=9 is 77.3%
CV accuracy estimate for k=12 is 76.0%
```