lecture2-supervised-learning

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1 Lecture 2: Supervised Machine Learning

1.0.1 Applied Machine Learning

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2 Announcements

- The linear algebra and probability tutorial is this week
  - Wednesday at 8pm
  - In Bloomberg 161
- The Python and Numpy tutorial is next week
  - Tuesday at 7:30pm
  - Room TBD

- Homework 0 is out on Gradescope

3 Recall: Supervised Learning

The most common approach to machine learning is supervised learning.

1. First, we collect a dataset of labeled training examples.
2. We train a model to output accurate predictions on this dataset.
3. When the model sees new, similar data, it will also be accurate.

4 Part 1: A Supervised Machine Learning Problem

Let's start by dissecting a simple example of a supervised learning problem.

5 Three Components of Supervised Machine Learning

To apply supervised learning, we define a dataset and a learning algorithm.

$$\text{Dataset} + \text{Learning Algorithm} \rightarrow \text{Predictive Model}$$

The output is a predictive model that maps inputs to targets. For instance, it can predict targets on new inputs.

6   A Supervised Learning Dataset

Let's start with a simple example of a supervised learning problem: predicting diabetes risk.

We start with a dataset of diabetes patients. * For each patient we have a access to their BMI and an estimate of diabetes risk (from 0-400). * We are interested in understanding how BMI affects an individual's diabetes risk.

```python
[2]: import numpy as np
     import pandas as pd
     from sklearn import datasets

     # We will use the UCI Diabetes Dataset
     # It's a toy dataset often used to demo ML algorithms.
     diabetes_X, diabetes_y = datasets.load_diabetes(return_X_y=True, as_frame=True)

     # Use only the BMI feature
     diabetes_X = diabetes_X.loc[:, ['bmi']]

     # The BMI is zero-centered and normalized; we recenter it for ease of␣
      ↪presentation
     diabetes_X = diabetes_X * 30 + 25

     # Collect 20 data points
     diabetes_X_train = diabetes_X.iloc[-20:]
     diabetes_y_train = diabetes_y.iloc[-20:]

     # Display some of the data points
     pd.concat([diabetes_X_train, diabetes_y_train], axis=1).head()
```

```
[2]:            bmi  target
     422  27.335902   233.0
     423  23.811456    91.0
     424  25.331171   111.0
     425  23.779122   152.0
     426  23.973128   120.0
```

We can also visualize this two-dimensional dataset.

```python
[3]: %matplotlib inline
     import matplotlib.pyplot as plt
     plt.rcParams['figure.figsize'] = [12, 4]

     plt.scatter(diabetes_X_train, diabetes_y_train,  color='black')
     plt.xlabel('Body Mass Index (BMI)')
     plt.ylabel('Diabetes Risk')
```

```
[3]: Text(0, 0.5, 'Diabetes Risk')
```
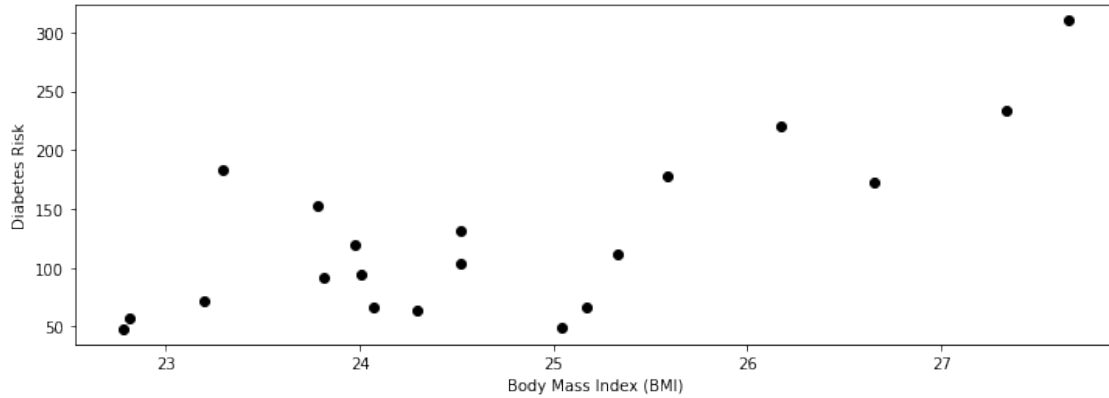
7 A Supervised Learning Algorithm: The Model Class

Let's assume that risk is a linear function of BMI. In other words, for some unknown $\theta_0, \theta_1 \in \mathbb{R}$, we have
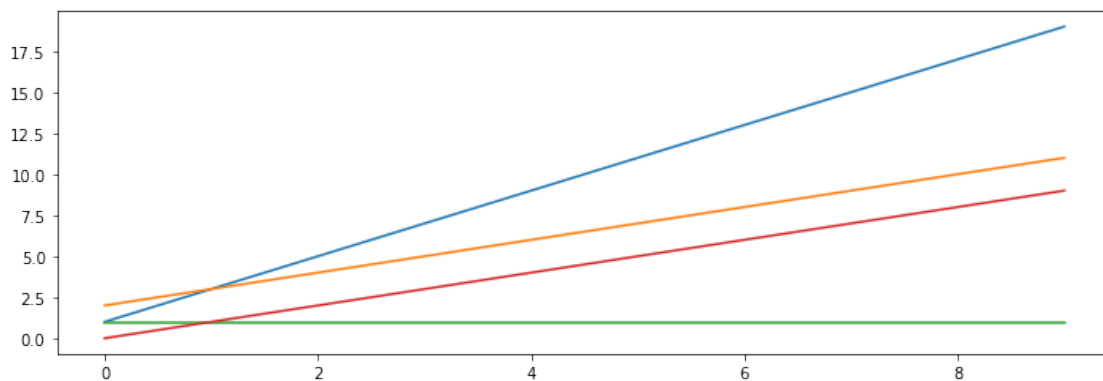
$$y = \theta_1 \cdot x + \theta_0,$$

where x is the BMI (also called the independent variable), and y is the diabetes risk score (the dependent variable).

The parameters θ_1, θ_0 are the slope and the intercept of the line relates x to y.

We can visualize this for a few values of θ_1, θ_0.

```
[4]: theta_list = [(1, 2), (2,1), (1,0), (0,1)]
for theta0, theta1 in theta_list:
    x = np.arange(10)
    y = theta1 * x + theta0
    plt.plot(x,y)
```

8 A Supervised Learning Algorithm: The Optimizer

Given our assumption that x, y follow the a linear relationship, the goal of a supervised learning algorithm is to find a good set of parameters consistent with the data.

This is an optimization problem.

For now, let's call the `sklearn.linear_model` library to find a θ_1, θ_0 that fit the data well.

```python
[6]: from sklearn import linear_model
     from sklearn.metrics import mean_squared_error

     # Create linear regression object
     regr = linear_model.LinearRegression()

     # Train the model using the training sets
     regr.fit(diabetes_X_train, diabetes_y_train.values)

     # Make predictions on the training set
     diabetes_y_train_pred = regr.predict(diabetes_X_train)

     # The coefficients
     print('Slope (theta1): \t', regr.coef_[0])
     print('Intercept (theta0): \t', regr.intercept_)
```

```
Slope (theta1):          37.378842160517664
Intercept (theta0):      -797.0817390342369
```

9 A Supervised Learning Model

The supervised learning algorithm gave us a pair of parameters θ_1^*, θ_0^*. These define the *predictive model f^**, defined as
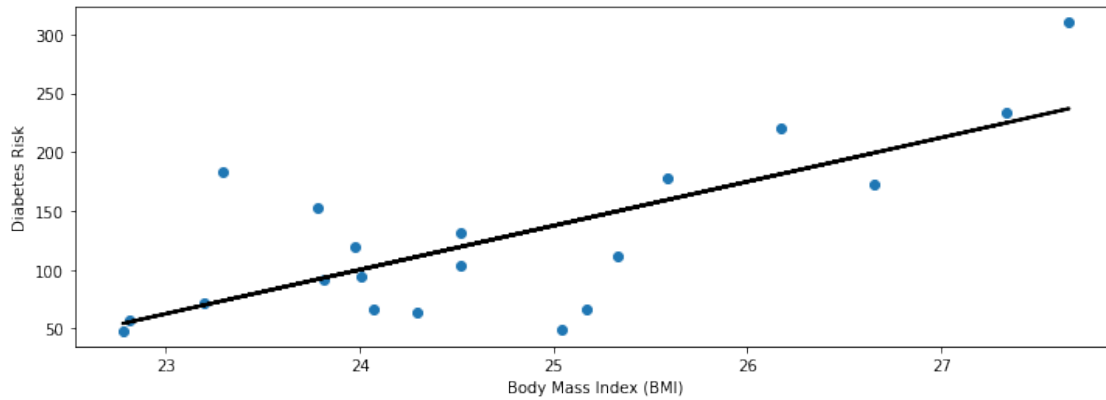
$$f(x) = \theta_1^* \cdot x + \theta_0^*,$$

where again x is the BMI, and y is the diabetes risk score.

We can visualize the linear model that best fits our data.

```python
[7]: plt.xlabel('Body Mass Index (BMI)')
     plt.ylabel('Diabetes Risk')
     plt.scatter(diabetes_X_train, diabetes_y_train)
     plt.plot(diabetes_X_train, diabetes_y_train_pred, color='black', linewidth=2)
```

```
[7]: [<matplotlib.lines.Line2D at 0x1253f9240>]
```

10 Making New Predictions

Given a new dataset of patients with a known BMI, we can use this model to estimate their diabetes risk.

Given an x_{new}, we can output prediction y_{new} as

$$y_{\text{new}} = f(x_{\text{new}}) = \theta_1^* \cdot x_{\text{new}} + \theta_0.$$

Let's start by loading more data. We will load three new patients (shown in red below) that we haven't seen before.

```
[8]: # Collect 3 data points
     diabetes_X_test = diabetes_X.iloc[:3]
     diabetes_y_test = diabetes_y.iloc[:3]

     plt.scatter(diabetes_X_train, diabetes_y_train)
     plt.scatter(diabetes_X_test, diabetes_y_test,  color='red')
     plt.xlabel('Body Mass Index (BMI)')
     plt.ylabel('Diabetes Risk')
     plt.legend(['Initial patients', 'New patients'])
```

[8]: <matplotlib.legend.Legend at 0x1259cd390>
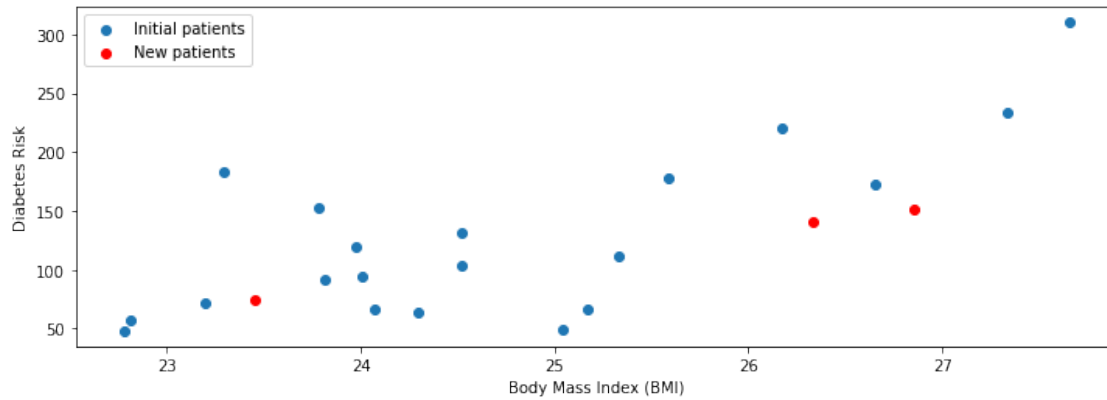
Our linear model provides an estimate of the diabetes risk for these patients.

```
[9]: # generate predictions on the new patients
     diabetes_y_test_pred = regr.predict(diabetes_X_test)

     # visualize the results
     plt.xlabel('Body Mass Index (BMI)')
     plt.ylabel('Diabetes Risk')
     plt.scatter(diabetes_X_train, diabetes_y_train)
     plt.scatter(diabetes_X_test, diabetes_y_test, color='red', marker='o')
     plt.plot(diabetes_X_train, diabetes_y_train_pred, color='black', linewidth=1)
     plt.plot(diabetes_X_test, diabetes_y_test_pred, 'x', color='red', mew=3,␣
      ↪markersize=8)
     plt.legend(['Model', 'Prediction', 'Initial patients', 'New patients'])
```

[9]: <matplotlib.legend.Legend at 0x125bfb048>

6
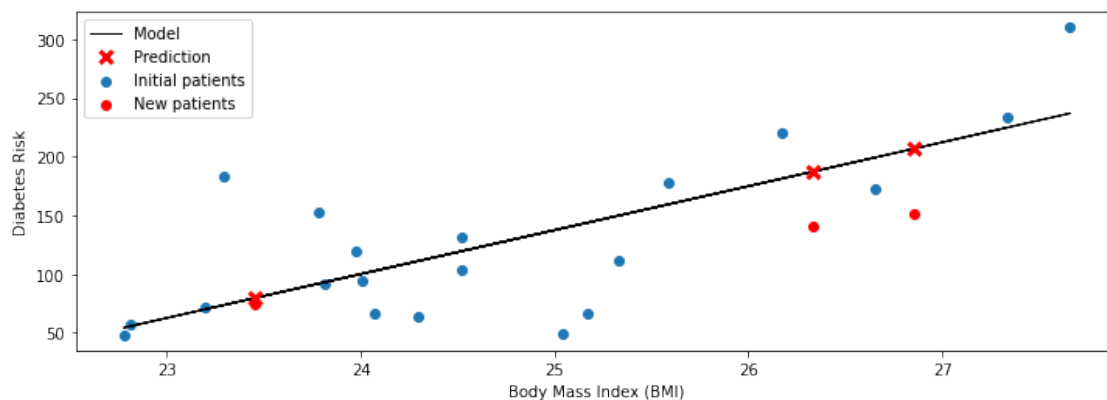
11 Why Supervised Learning?

Supervised learning can be useful in many ways. * Making predictions on new data. * Understanding the mechanisms through which input variables affect targets.

12 Applications of Supervised Learning

Many of the most important applications of machine learning are supervised: * Classifying medical images. * Translating between pairs of languages. * Detecting objects in a self-driving car.

Part 2: Anatomy of a Supervised Learning Problem: The Dataset

We have seen an example of supervised machine learning.

Let's now examine more closely the components of a supervised learning problem, starting with the dataset.

13 Recall: Three Components of a Supervised Machine Learning Problem

To apply supervised learning, we define a dataset and a learning algorithm.

$$\text{Dataset} + \text{Learning Algorithm} \rightarrow \text{Predictive Model}$$

The output is a predictive model that maps inputs to targets. For instance, it can predict targets on new inputs.

14 A Supervised Learning Dataset

Let's dive deeper into what's a supervised learning dataset.

We will again use the UCI Diabetes Dataset as our example.

The UCI dataset contains many additional data columns besides `bmi`, including age, sex, and blood pressure. We can ask `sklearn` to give us more information about this dataset.

```python
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
plt.rcParams['figure.figsize'] = [12, 4]
from sklearn import datasets

# Load the diabetes dataset
diabetes = datasets.load_diabetes(as_frame=True)
print(diabetes.DESCR)
```

```
.. _diabetes_dataset:

Diabetes dataset
```

Ten baseline variables, age, sex, body mass index, average blood
pressure, and six blood serum measurements were obtained for each of n =
442 diabetes patients, as well as the response of interest, a
quantitative measure of disease progression one year after baseline.

Data Set Characteristics:

  :Number of Instances: 442

  :Number of Attributes: First 10 columns are numeric predictive values

  :Target: Column 11 is a quantitative measure of disease progression one year
after baseline

  :Attribute Information:
      - age   age in years
      - sex
      - bmi   body mass index
      - bp   average blood pressure
      - s1   tc, T-Cells (a type of white blood cells)
      - s2   ldl, low-density lipoproteins
      - s3   hdl, high-density lipoproteins
      - s4   tch, thyroid stimulating hormone
      - s5   ltg, lamotrigine
      - s6   glu, blood sugar level

Note: Each of these 10 feature variables have been mean centered and scaled by
the standard deviation times `n_samples` (i.e. the sum of squares of each column
totals 1).

Source URL:
https://www4.stat.ncsu.edu/~boos/var.select/diabetes.html

For more information see:
Bradley Efron, Trevor Hastie, Iain Johnstone and Robert Tibshirani (2004) "Least
Angle Regression," Annals of Statistics (with discussion), 407-499.
(https://web.stanford.edu/~hastie/Papers/LARS/LeastAngle_2002.pdf)

15 A Supervised Learning Dataset: Notation

We say that a training dataset of size n (e.g., n patients) is a set

$$\mathcal{D} = \{(x^{(i)}, y^{(i)}) \mid i = 1, 2, ..., n\}$$

Each $x^{(i)}$ denotes an input (e.g., the measurements for patient i), and each $y^{(i)} \in \mathcal{Y}$ is a target
(e.g., the diabetes risk).

Together, $(x^{(i)}, y^{(i)})$ form a *training example*.

We can look at the diabetes dataset in this form.

```
[11]: # Load the diabetes dataset
      diabetes_X, diabetes_y = diabetes.data, diabetes.target

      # Print part of the dataset
      diabetes_X.head()
```

```
[11]:         age       sex       bmi        bp        s1        s2        s3  \
      0   0.038076  0.050680  0.061696  0.021872 -0.044223 -0.034821 -0.043401
      1  -0.001882 -0.044642 -0.051474 -0.026328 -0.008449 -0.019163  0.074412
      2   0.085299  0.050680  0.044451 -0.005671 -0.045599 -0.034194 -0.032356
      3  -0.089063 -0.044642 -0.011595 -0.036656  0.012191  0.024991 -0.036038
      4   0.005383 -0.044642 -0.036385  0.021872  0.003935  0.015596  0.008142

               s4        s5        s6
      0  -0.002592  0.019908 -0.017646
      1  -0.039493 -0.068330 -0.092204
      2  -0.002592  0.002864 -0.025930
      3   0.034309  0.022692 -0.009362
      4  -0.002592 -0.031991 -0.046641
```

16 Training Dataset: Inputs

More precisely, an input $x^{(i)} \in \mathcal{X}$ is a d-dimensional vector of the form

$$x^{(i)} = \begin{bmatrix} x_1^{(i)} \\ x_2^{(i)} \\ \vdots \\ x_d^{(i)} \end{bmatrix}$$

For example, it could be the values of the d features for patient i.

The set $\mathcal{X}$ is called the feature space. Often, we have, $\mathcal{X} = \mathbb{R}^d$.

Let's look at data for one patient.

```
[12]: diabetes_X.iloc[0]
```

```
[12]: age    0.038076
      sex    0.050680
      bmi    0.061696
      bp     0.021872
      s1    -0.044223
      s2    -0.034821
      s3    -0.043401
      s4    -0.002592
```

```
s5      0.019908
s6     -0.017646
Name: 0, dtype: float64
```

17 Training Dataset: Attributes

We refer to the numerical variables describing the patient as *attributes*. Examples of attributes include: * The age of a patient. * The patient's gender. * The patient's BMI.

Note that thes attributes in the above example have been mean-centered at zero and re-scaled to have a variance of one.

18 Training Dataset: Features

Often, an input object has many attributes, and we want to use these attributes to define more complex descriptions of the input.

- Is the patient old and a man? (Useful if old men are at risk).
- Is the BMI above the obesity threshold?

We call these custom attributes *features*.

Let's create an "old man" feature.

```
[13]: diabetes_X['old_man'] = (diabetes_X['sex'] > 0) & (diabetes_X['age'] > 0.05)
      diabetes_X.head()
```

```
[13]:         age       sex       bmi        bp        s1        s2        s3  \
      0  0.038076  0.050680  0.061696  0.021872 -0.044223 -0.034821 -0.043401
      1 -0.001882 -0.044642 -0.051474 -0.026328 -0.008449 -0.019163  0.074412
      2  0.085299  0.050680  0.044451 -0.005671 -0.045599 -0.034194 -0.032356
      3 -0.089063 -0.044642 -0.011595 -0.036656  0.012191  0.024991 -0.036038
      4  0.005383 -0.044642 -0.036385  0.021872  0.003935  0.015596  0.008142


               s4        s5        s6  old_man
      0 -0.002592  0.019908 -0.017646    False
      1 -0.039493 -0.068330 -0.092204    False
      2 -0.002592  0.002864 -0.025930     True
      3  0.034309  0.022692 -0.009362    False
      4 -0.002592 -0.031991 -0.046641    False
```

19   Training Dataset: Features

We may denote features via a function $\phi : \mathcal{X} \to \mathbb{R}^p$ that takes an input $x^{(i)} \in \mathcal{X}$ and outputs a p-dimensional vector

$$\phi(x^{(i)}) = \begin{bmatrix} \phi(x^{(i)})_1 \\ \phi(x^{(i)})_2 \\ \vdots \\ \phi(x^{(i)})_p \end{bmatrix}$$

We say that $\phi(x^{(i)})$ is a *featurized* input, and each $\phi(x^{(i)})_j$ is a *feature*.

20   Features vs Attributes

In practice, the terms attribute and features are often used interchangeably. Most authors refer to $x^{(i)}$ as a vector of features.

We will follow this convention and use the term "attribute" only when there is ambiguity between features and attributes.
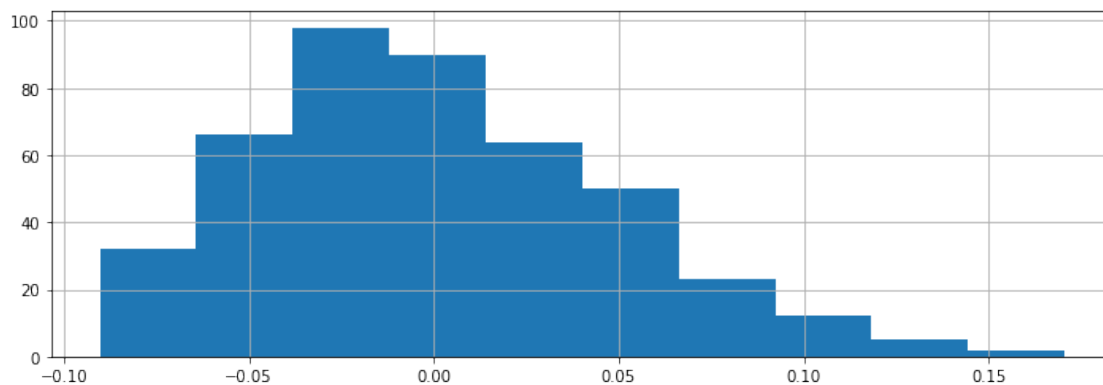
21   Features: Discrete vs. Continuous

Features can be either discrete or continuous. We will see that some ML algorthims handle these differently.

The BMI feature that we have seen earlier is an example of a continuous feature.

We can visualize its distribution.

```
[14]: diabetes_X.loc[:, 'bmi'].hist()
```
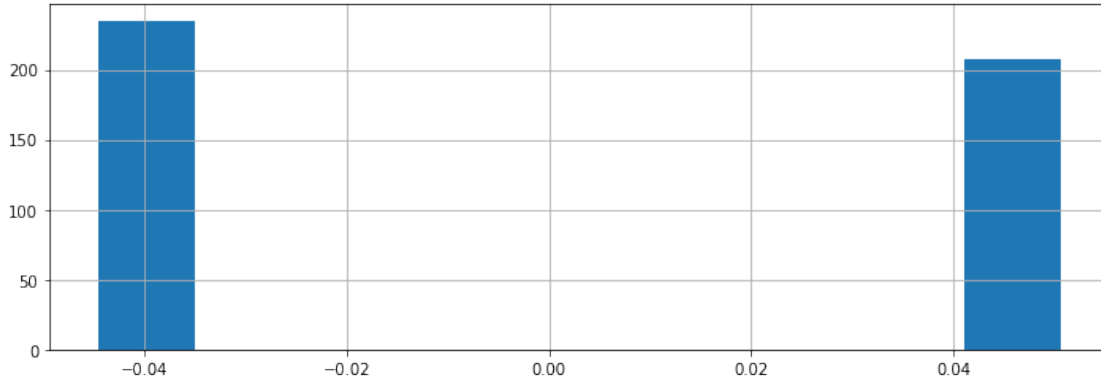
[14]: <AxesSubplot:>

Other features take on one of a finite number of discrete values. The `sex` column is an example of a categorical feature.

In this example, the dataset has been pre-processed such that the two values happen to be 0.05068012 and -0.04464164.

```
[15]: print(diabetes_X.loc[:, 'sex'].unique())
      diabetes_X.loc[:, 'sex'].hist()
```

```
[ 0.05068012 -0.04464164]
```

```
[15]: <AxesSubplot:>
```


22   Training Dataset: Targets

For each patient, we are interested in predicting a quantity of interest, the *target*. In our example, this is the patient's diabetes risk.

Formally, when $(x^{(i)}, y^{(i)})$ form a *training example*, each $y^{(i)} \in \mathcal{Y}$ is a target. We call $\mathcal{Y}$ the target space.

We plot the distirbution of risk scores below.

```
[16]: plt.xlabel('Diabetes risk score')
      plt.ylabel('Number of patients')
      diabetes_y.hist()
```

```
[16]: <AxesSubplot:xlabel='Diabetes risk score', ylabel='Number of patients'>
```
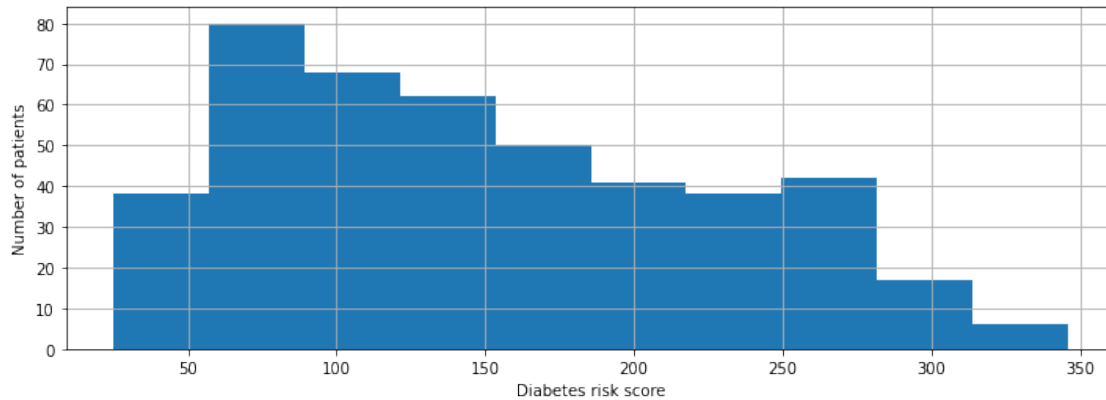
23 Targets: Regression vs. Classification

We distinguish between two broad types of supervised learning problems that differ in the form of the target variable.

1. **Regression**: The target variable y is continuous. We are fitting a curve in a high-dimensional feature space that approximates the shape of the dataset.
2. **Classification**: The target variable y is discrete. Each discrete value corresponds to a *class* and we are looking for a hyperplane that separates the different classes.

We can easily turn our earlier regression example into classification by discretizing the diabetes risk scores into high or low.

```
[17]: # Discretize the targets
      diabetes_y_train_discr = np.digitize(diabetes_y_train, bins=[150])

      # Visualize it
      plt.scatter(diabetes_X_train[diabetes_y_train_discr==0],␣
       ↪diabetes_y_train[diabetes_y_train_discr==0], marker='o', s=80,␣
       ↪facecolors='none', edgecolors='g')
      plt.scatter(diabetes_X_train[diabetes_y_train_discr==1],␣
       ↪diabetes_y_train[diabetes_y_train_discr==1], marker='o', s=80,␣
       ↪facecolors='none', edgecolors='r')
      plt.legend(['Low-Risk Patients', 'High-Risk Patients'])
```

```
[17]: <matplotlib.legend.Legend at 0x125ffc240>
```
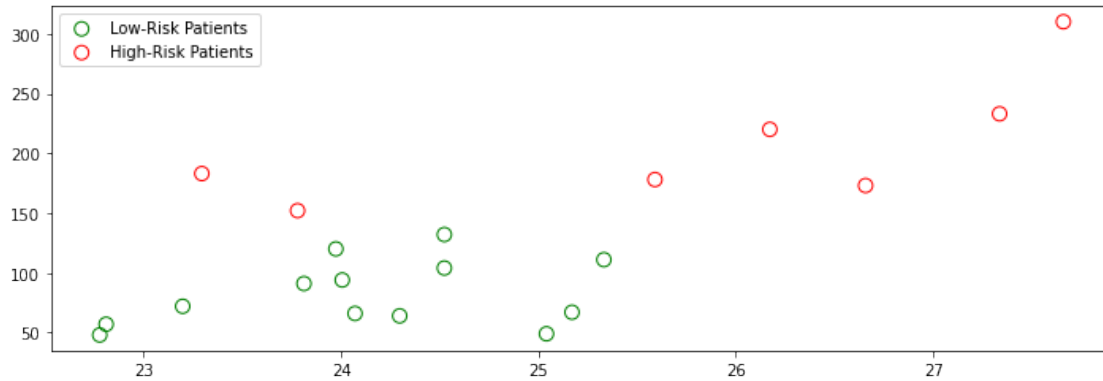
Let's try to generate predictions for this dataset.

```
[18]: # Create logistic regression object (note: this is actually a classification
      →algorithm!)
      clf = linear_model.LogisticRegression()

      # Train the model using the training sets
      clf.fit(diabetes_X_train, diabetes_y_train_discr)

      # Make predictions on the training set
      diabetes_y_train_pred = clf.predict( )

      # Visualize it
      plt.scatter(diabetes_X_train[diabetes_y_train_discr==0],
       →diabetes_y_train[diabetes_y_train_discr==0], marker='o', s=140,
       →facecolors='none', edgecolors='g')
      plt.scatter(diabetes_X_train[diabetes_y_train_discr==1],
       →diabetes_y_train[diabetes_y_train_discr==1], marker='o', s=140,
       →facecolors='none', edgecolors='r')
      plt.scatter(diabetes_X_train[diabetes_y_train_pred==0],
       →diabetes_y_train[diabetes_y_train_pred==0], color='g', s=20)
      plt.scatter(diabetes_X_train[diabetes_y_train_pred==1],
       →diabetes_y_train[diabetes_y_train_pred==1], color='r', s=20)
      plt.legend(['Low-Risk Patients', 'High-Risk Patients', 'Low-Risk Predictions',
       →'High-Risk Predictions'])
```

```
[18]: <matplotlib.legend.Legend at 0x11847d320>
```

14
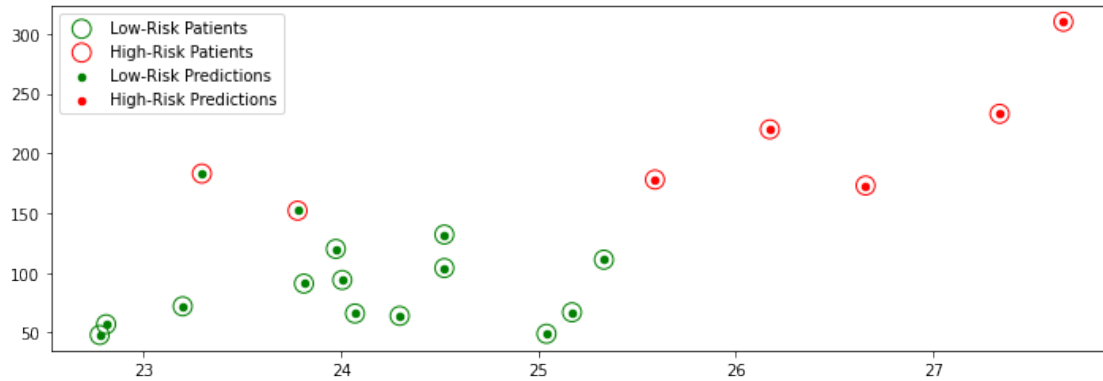
Part 3: Anatomy of a Supervised Learning Problem: The Learning Algorithm

Let's now look at what a general supervised learning algorithm looks like.

24 Recall: Three Components of a Supervised Machine Learning Problem

To apply supervised learning, we define a dataset and a learning algorithm.

$$\text{Dataset} + \text{Learning Algorithm} \rightarrow \text{Predictive Model}$$

The output is a predictive model that maps inputs to targets. For instance, it can predict targets on new inputs.

25 The Components of a Supervised Machine Learning Algorithm

We can also define the high-level structure of a supervised learning algorithm as consisting of three components: * A **model class**: the set of possible models we consider. * An **objective** function, which defines how good a model is. * An **optimizer**, which finds the best predictive model in the model class according to the objective function

Let's look again at our diabetes dataset for an example.

```python
[19]: import numpy as np
import pandas as pd
from sklearn import datasets
import matplotlib.pyplot as plt
plt.rcParams['figure.figsize'] = [12, 4]

# Load the diabetes dataset
diabetes = datasets.load_diabetes(as_frame=True)
diabetes_X, diabetes_y = diabetes.data, diabetes.target
```

```
# Print part of the dataset
diabetes_X.head()
```

[19]:
```
        age       sex       bmi        bp        s1        s2        s3  \
0  0.038076  0.050680  0.061696  0.021872 -0.044223 -0.034821 -0.043401
1 -0.001882 -0.044642 -0.051474 -0.026328 -0.008449 -0.019163  0.074412
2  0.085299  0.050680  0.044451 -0.005671 -0.045599 -0.034194 -0.032356
3 -0.089063 -0.044642 -0.011595 -0.036656  0.012191  0.024991 -0.036038
4  0.005383 -0.044642 -0.036385  0.021872  0.003935  0.015596  0.008142


         s4        s5        s6
0 -0.002592  0.019908 -0.017646
1 -0.039493 -0.068330 -0.092204
2 -0.002592  0.002864 -0.025930
3  0.034309  0.022692 -0.009362
4 -0.002592 -0.031991 -0.046641
```

26 Model: Notation

We'll say that a model is a function

$$f : \mathcal{X} \rightarrow \mathcal{Y}$$

that maps inputs $x \in \mathcal{X}$ to targets $y \in \mathcal{Y}$.

Often, models have *parameters* $\theta \in \Theta$ living in a set Θ. We will then write the model as

$$f_\theta : \mathcal{X} \rightarrow \mathcal{Y}$$

to denote that it's parametrized by θ.

27 Model Class: Notation

Formally, the model class is a set

$$\mathcal{M} \subseteq \{f \mid f : \mathcal{X} \rightarrow \mathcal{Y}\}$$

of possible models that map input features to targets.

When the models f_θ are paremetrized by *parameters* $\theta \in \Theta$ living in some set Θ. Thus we can also write

$$\mathcal{M} = \{f_\theta \mid \theta \in \Theta\}.$$

28 Model Class: Example

One simple approach is to assume that x and y are related by a linear model of the form

$$y = \theta_0 + \theta_1 \cdot x_1 + \theta_2 \cdot x_2 + \ldots + \theta_d \cdot x_d$$

where x is a featurized input and y is the target.

The θ_j are the *parameters* of the model, $\Theta = \mathbb{R}^{d+1}$, and $\mathcal{M} = \{\theta_0 + \theta_1 \cdot x_1 + \theta_2 \cdot x_2 + \ldots + \theta_d \cdot x_d \mid \theta \in \mathbb{R}^{d+1}\}$

29 Objectives: Notation

To capture this intuition, we define an *objective function* (also called a *loss function*)

$$J(f) : \mathcal{M} \to [0, \infty),$$

which describes the extent to which f "fits" the data $\mathcal{D} = \{(x^{(i)}, y^{(i)}) \mid i = 1, 2, ..., n\}$.

When f is parametrized by $\theta \in \Theta$, the objective becomes a function $J(\theta) : \Theta \to [0, \infty)$.

30 Objective: Examples

What would are some possible objective functions? We will see many, but here are a few examples:
* Mean squared error:

$$J(\theta) = \frac{1}{2n} \sum_{i=1}^{n} \left(f_\theta(x^{(i)}) - y^{(i)} \right)^2$$

* Absolute (L1) error:

$$J(\theta) = \frac{1}{n} \sum_{i=1}^{n} \left| f_\theta(x^{(i)}) - y^{(i)} \right|$$

These are defined for a dataset $\mathcal{D} = \{(x^{(i)}, y^{(i)}) \mid i = 1, 2, ..., n\}$.

```
[60]: from sklearn.metrics import mean_squared_error, mean_absolute_error

      y1 = np.array([1, 2, 3, 4])
      y2 = np.array([-1, 1, 3, 5])

      print('Mean squared error: %.2f' % mean_squared_error(y1, y2))
      print('Mean absolute error: %.2f' % mean_absolute_error(y1, y2))
```

```
Mean squared error: 1.50
Mean absolute error: 1.00
```

31 Optimizer: Notation

At a high-level an optimizer takes an objective J and a model class $\mathcal{M}$ and finds a model $f \in \mathcal{M}$ with the smallest value of the objective J.

$$\min_{f \in \mathcal{M}} J(f)$$

Intuitively, this is the function that bests "fits" the data on the training dataset.

When f is parametrized by $\theta \in \Theta$, the optimizer minimizes a function $J(\theta)$ over all $\theta \in \Theta$.

32 Optimizer: Example

We will see that behind the scenes, the `sklearn.linear_models.LinearRegression` algorithm optimizes the MSE loss.

$$\min_{\theta \in \mathbb{R}} \frac{1}{2n} \sum_{i=1}^{n} \left(f_\theta(x^{(i)}) - y^{(i)} \right)^2$$

We can easily measure the quality of the fit on the training set and the test set.

Let's run the above algorithm on our diabetes dataset.

```
[54]: # Collect 20 data points for training
      diabetes_X_train = diabetes_X.iloc[-20:]
      diabetes_y_train = diabetes_y.iloc[-20:]

      # Create linear regression object
      regr = linear_model.LinearRegression()

      # Train the model using the training sets
      regr.fit(diabetes_X_train, diabetes_y_train.values)

      # Make predictions on the training set
      diabetes_y_train_pred = regr.predict(diabetes_X_train)

      # Collect 3 data points for testing
      diabetes_X_test = diabetes_X.iloc[:3]
      diabetes_y_test = diabetes_y.iloc[:3]

      # generate predictions on the new patients
      diabetes_y_test_pred = regr.predict(diabetes_X_test)
```

The algorithm returns a predictive model. We can visualize its predictions below.

```
[55]: # visualize the results
      plt.xlabel('Body Mass Index (BMI)')
      plt.ylabel('Diabetes Risk')
      plt.scatter(diabetes_X_train.loc[:, ['bmi']], diabetes_y_train)
      plt.scatter(diabetes_X_test.loc[:, ['bmi']], diabetes_y_test, color='red',␣
       ↪marker='o')
      # plt.scatter(diabetes_X_train.loc[:, ['bmi']], diabetes_y_train_pred,␣
       ↪color='black', linewidth=1)
      plt.plot(diabetes_X_test.loc[:, ['bmi']], diabetes_y_test_pred, 'x',␣
       ↪color='red', mew=3, markersize=8)
      plt.legend(['Model', 'Prediction', 'Initial patients', 'New patients'])
```

```
[55]: <matplotlib.legend.Legend at 0x12f6a46a0>
```
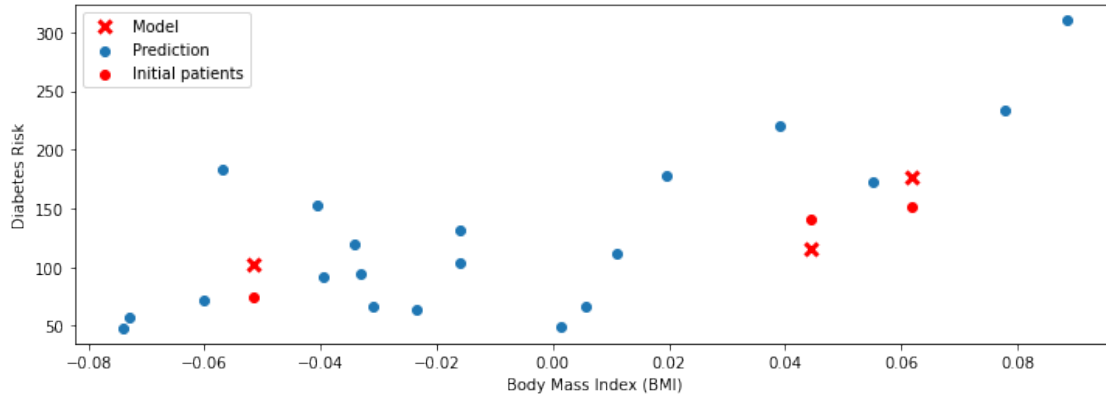
```
[59]: from sklearn.metrics import mean_squared_error

      print('Training set mean squared error: %.2f'
            % mean_squared_error(diabetes_y_train, diabetes_y_train_pred))
      print('Test set mean squared error: %.2f'
            % mean_squared_error(diabetes_y_test, diabetes_y_test_pred))
      print('Test set mean squared error on random inputs: %.2f'
            % mean_squared_error(diabetes_y_test, np.random.
      ↪randn(*diabetes_y_test_pred.shape)))
```

```
Training set mean squared error: 1118.22
Test set mean squared error: 667.81
Test set mean squared error on random inputs: 15887.97
```

33 Summary: Components of a Supervised Machine Learning Problem

To apply supervised learning, we define a dataset and a learning algorithm.

$$\underbrace{\text{Dataset}}_{\text{Features, Attributes, Targets}} + \underbrace{\text{Learning Algorithm}}_{\text{Model Class + Objective + Optimizer}} \rightarrow \text{Predictive Model}$$

The output is a predictive model that maps inputs to targets. For instance, it can predict targets on new inputs.

34 Notation: Feature Matrix

Suppose that we have a dataset of size n (e.g., n patients), indexed by $i = 1, 2, ..., n$. Each $x^{(i)}$ is a vector of d features.

Feature Matrix   Machine learning algorithms are most easily defined in the language of linear algebra. Therefore, it will be useful to represent the entire dataset as one matrix $X \in \mathbb{R}^{n \times d}$, of the form:

$$X = \begin{bmatrix} x_1^{(1)} & x_1^{(2)} & \dots & x_1^{(n)} \\ x_2^{(1)} & x_2^{(2)} & \dots & x_2^{(n)} \\ \vdots & & & \\ x_d^{(1)} & x_d^{(2)} & \dots & x_d^{(n)} \end{bmatrix}.$$

Similarly, we can vectorize the target variables into a vector $y \in \mathbb{R}^n$ of the form

$$y = \begin{bmatrix} x^{(1)} \\ x^{(2)} \\ \vdots \\ x^{(n)} \end{bmatrix}.$$