MTH 221

Fundamentals of Machine Learning

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Lecture 5: Linear Regression & Gradient Descent & Logistic Regression

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Recap on Naive Bayes

Setting: binary classification w/ dataset $\{x_i, y_i\}_{i=1}^n, (x_i, y_i) \sim P,$ where $x \in \mathbb{R}^d, y \in \{-1,1\}$

Goal: estimate $P(y \mid x)$

We take a **generative modeling** approach here:

$$P(y \mid x) \propto P(x \mid y)P(y)$$

Estimate $P(x \mid y)$ & $P(y)$ from data
(hence generative modeling)

(Discriminative modeling: directly estimate $P(y \mid x)$)

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Recap on Naive Bayes

Estimate $P(y)$ from data:

$$P(y \mid x) \propto P(x \mid y)P(y)$$

Estimate $P(y)$ is easy:

$$P(y = 1) \approx \frac{\sum_{i=1}^{n} \mathbf{1}(y_i = 1)}{n}$$

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Recap on Naive Bayes

Estimate $P(x \mid y)$ from data:

$$P(y \mid x) \propto P(x \mid y)P(y)$$

Estimate $P(x \mid y)$ is not easy:

x can be high-dimensional, e.g., d is large!

There may not be repetitions in $\{x_i\}_{i=1}^{n}$!

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Recap on Naive Bayes

The key assumption in Naive Bayes

The Naive Bayes assumption:

$$P(x \mid y) = \prod_{\alpha=1}^{d} P(x[\alpha] \mid y)$$

Conditioned on label y, feature values are **independent**!

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Recap on Naive Bayes

Once estimated $P(y)$ and $P(x \mid y)$, we can make prediction:

$$P(y \mid x) \propto P(x \mid y)P(y)$$

In test time, given x:

$$\hat{y} = \arg\max_y P(y \mid x)$$

$$= \arg\max_y P(x \mid y)P(y) = \arg\max_y \left(\prod_{\alpha=1}^{d} P(x[\alpha] \mid y)\right)P(y)$$

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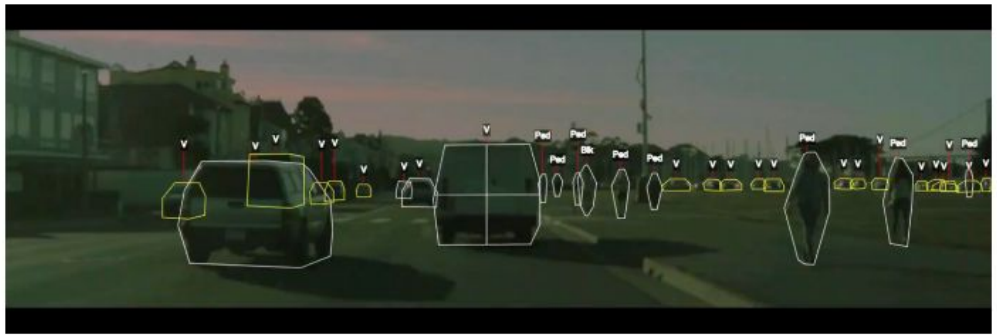
Plan for today

- Linear Regression
- Gradient Descent
- Logistic Regression

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.

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A Supervised Learning Dataset: Notation

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

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

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*.

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A Supervised Learning Dataset: Notation

We can look at the diabetes dataset in this form.

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

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

Out[11]:

	age	sex	bmi	bp	s1	s2	s3	s4	s5	s6
0	0.038076	0.050680	0.061696	0.021872	-0.044223	-0.034821	-0.043401	-0.002592	0.019908	-0.017646
1	-0.001882	-0.044642	-0.051474	-0.026328	-0.008449	-0.019163	0.074412	-0.039493	-0.068330	-0.092204
2	0.085299	0.050680	0.044451	-0.005671	-0.045599	-0.034194	-0.032356	-0.002592	0.002864	-0.025930
3	-0.089063	-0.044642	-0.011595	-0.036656	0.012191	0.024991	-0.036038	0.034309	0.022692	-0.009362
4	0.005383	-0.044642	-0.036385	0.021872	0.003935	0.015596	0.008142	-0.002592	-0.031991	-0.046641

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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 measurements the values of the d features for patient i.

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

Training Dataset: Inputs

Let's look at data for one patient.

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

```
Out[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
```

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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.

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Features: Discrete vs. Continuous

Features can be either discrete or continuous. We will see later that they may be handled differently by ML algorthims.

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Features: Discrete vs. Continuous

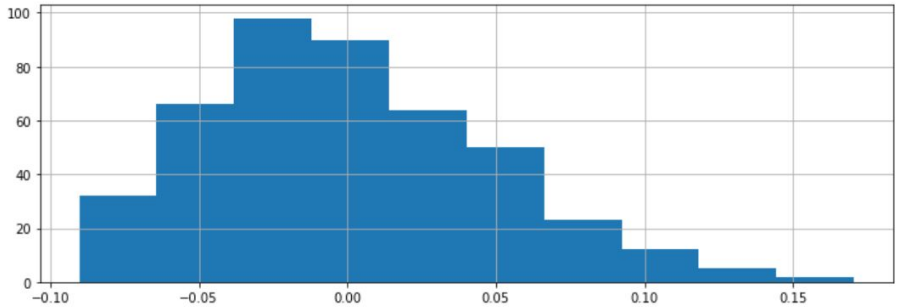
The BMI feature that we have seen earlier is an example of a continuous feature.

We can visualize its distribution.

Features ca may be handled differently

```
In [14]: diabetes_X.loc[:, 'bmi'].hist()

Out[14]: <AxesSubplot:>
```



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Features: Discrete vs. Continuous

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

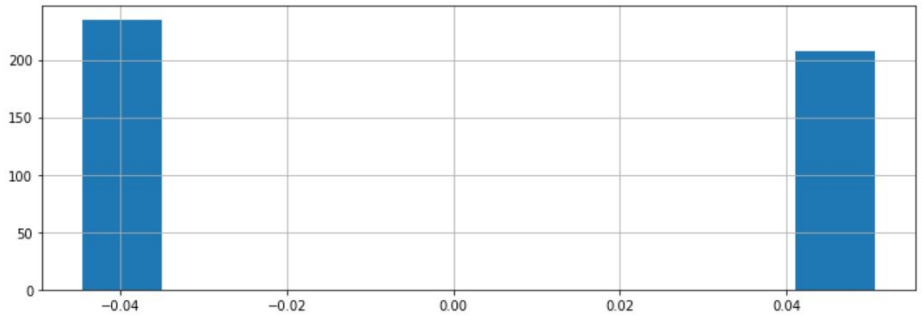
In this example, the dataset has been pre-processed such that the two values happen to be `0.05068012` and `-0.04464164`.

Features ca be handled differently

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

```
[ 0.05068012 -0.04464164]
```

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



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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.

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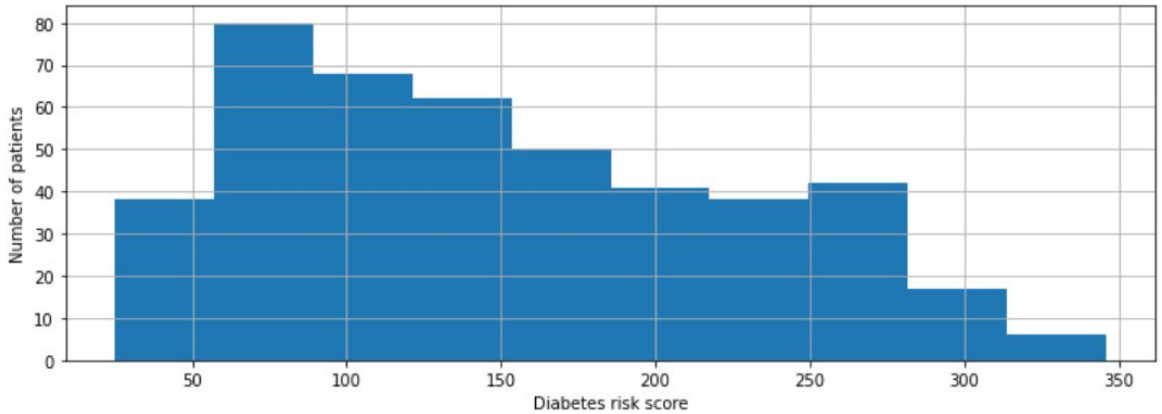
Training Dataset: Targets

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

Out[16]: <AxesSubplot:xlabel='Diabetes risk score', ylabel='Number of patients'>
```



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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.

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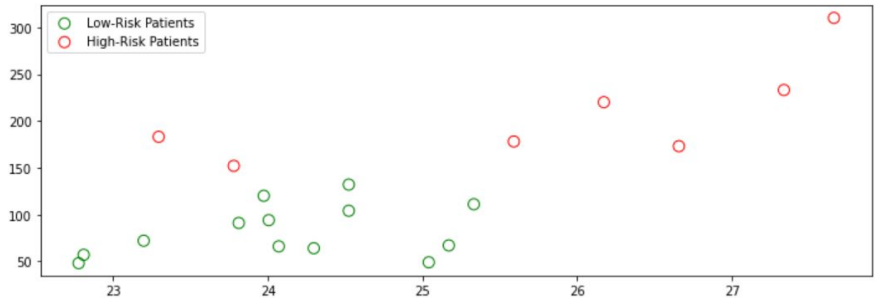
Targets: Regression vs. Classification

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

In [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[diabe
tes_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[diabe
tes_y_train_discr==1], marker='o', s=80, facecolors='none', edgecolors='r')
plt.legend(['Low-Risk Patients', 'High-Risk Patients'])
```

Out[17]:
```
<matplotlib.legend.Legend at 0x125ffc240>
```



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Let's try to generate predictions for this dataset.

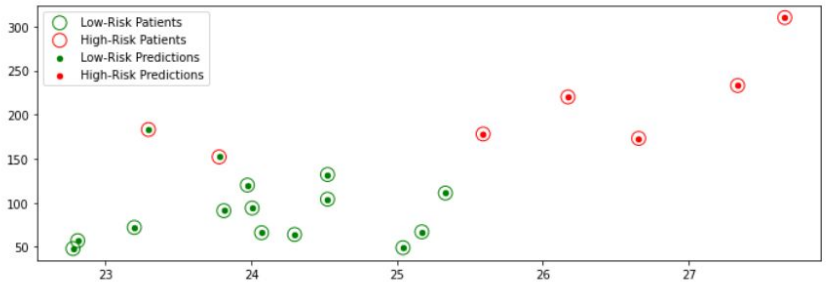
In [18]:
```
# Create logistic regression object (note: this is actually a classification al
gorithm!)
clf = linear_model.LogisticRegression()

# 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[diabe
tes_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[diabe
tes_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[diabet
es_y_train_pred==0], color='g', s=20)
plt.scatter(diabetes_X_train[diabetes_y_train_pred==1], diabetes_y_train[diabet
es_y_train_pred==1], color='r', s=20)
plt.legend(['Low-Risk Patients', 'High-Risk Patients', 'Low-Risk Predictions',
'High-Risk Predictions'])
```

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



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Components of Supervised Learning

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

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Model: Notation

We'll say that a model is a function

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

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

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

to denote that it's parametrized by θ.

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Model Class: Notation

Formally, the model class is a set

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

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

$$\mathcal{M} = \{f_\theta \mid f : \mathcal{X} \to \mathcal{Y};\ \theta \in \Theta\}.$$

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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 output and y is the target.

The θ_j are the *parameters* of the model.

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

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

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

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Objective: Examples

What would are some possible objective functions? We will see many, but here are a few

In [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
```

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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 $\theta \in \Theta$.

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Optimizer: Notation

We will use the a quadratic function as our running example for an objective J.

In [2]:
```
import numpy as np
import matplotlib.pyplot as plt
plt.rcParams['figure.figsize'] = [8, 4]
```

In [3]:
```
def quadratic_function(theta):
    """The cost function, J(theta)."""
    return 0.5*(2*theta-1)**2
```

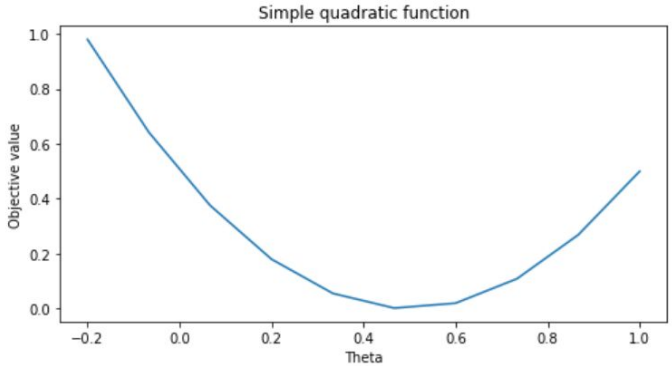
Optimizer: Notation

We can visualize it.

In [4]:
```
# First construct a grid of theta1 parameter pairs and their corresponding
# cost function values.
thetas = np.linspace(-0.2,1,10)
f_vals = quadratic_function(thetas[:,np.newaxis])

plt.plot(thetas, f_vals)
plt.xlabel('Theta')
plt.ylabel('Objective value')
plt.title('Simple quadratic function')
```

Out[4]:
```
Text(0.5, 1.0, 'Simple quadratic function')
```



Example Supervised ML Problem

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

Suppose we have a dataset of diabetes patients.

- For each patient we have a access to measurements from their medical record and an estimate of diabetes risk.
- We are interested in understanding how the measurements affect an individual's diabetes risk.

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A Supervised Learning Dataset

Let's return to our example: predicting diabates risk. What would a dataset look like?

We will use the UCI Diabetes Dataset; it's a toy dataset that's often used to demonstrate machine learning algorithms.

- For each patient we have a access to a measurement of their body mass index (BMI) and a quantiative diabetes risk score (from 0-400).
- We are interested in understanding how BMI affects an individual's diabetes risk.

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A Supervised Learning Dataset

Let's ret … ok like?

We will … emonstrate machine …

- F … s index (E …
- W … abetes risk.

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

# Load the diabetes dataset
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 presentat
ion
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()
```

Out[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

Slide Credit:

A Supervised Learning Dataset

We can also visualize this two-dimensional dataset.

Let's ret … k like?

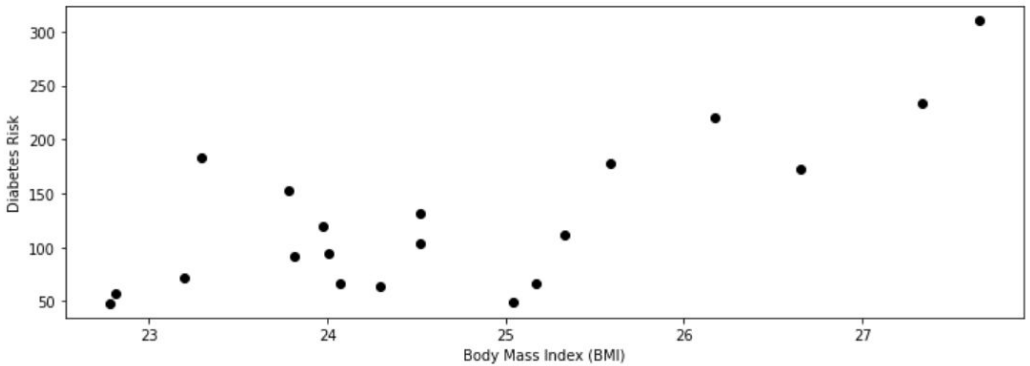
We will … monstrate machine …

- F … index (B …
- V … betes risk.

In [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')
```

Out[3]:
```
Text(0, 0.5, 'Diabetes Risk')
```



Slide Credit:

A Supervised Learning Algorithm

What is the relationship between BMI and diabetes risk?

We could 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 dependent variable), and y is the diabetes risk score (the independent variable).

Note that θ_1, θ_0 are the slope and the intercept of the line relates x to y. We call them *parameters*.

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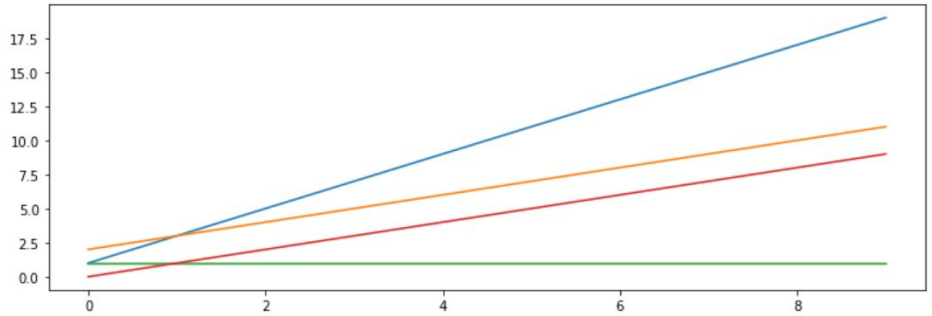
A Supervised Learning Algorithm

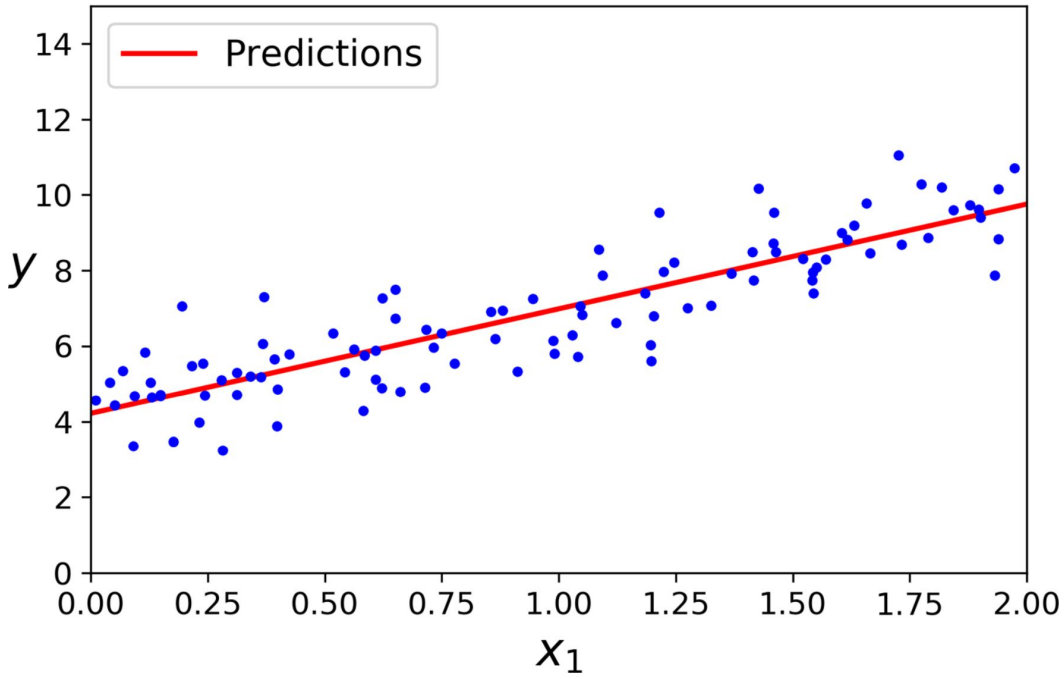
We can visualize this for a few values of θ_1, θ_0.

In [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)
```



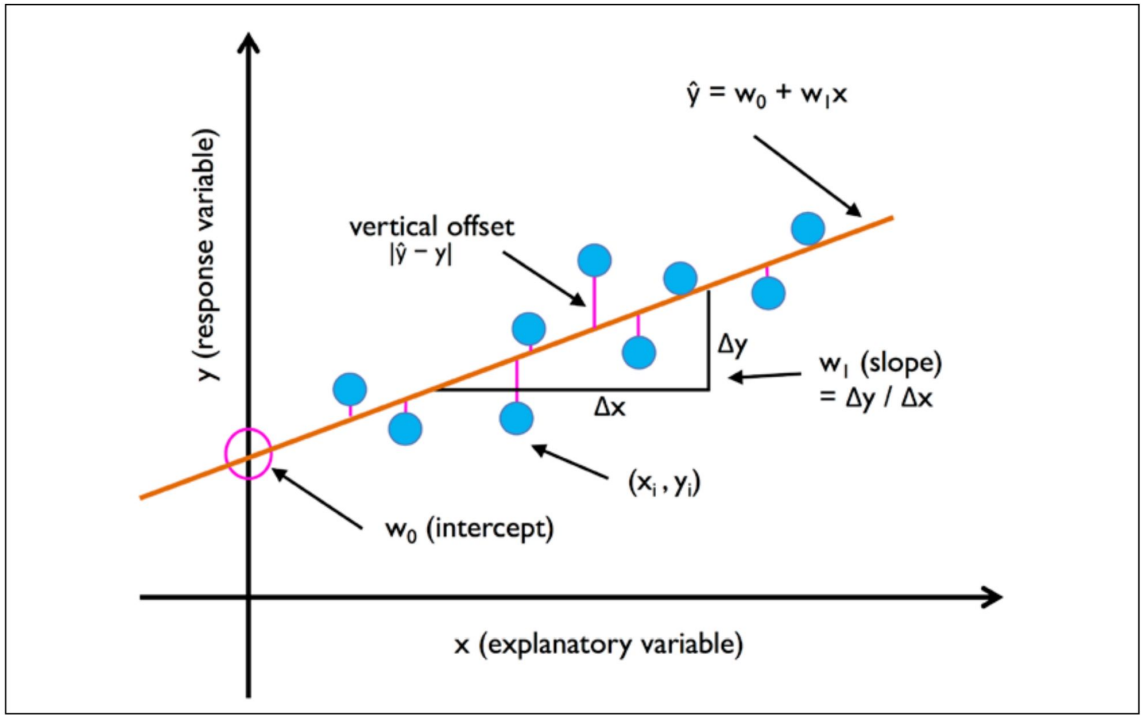
Slide Credit: Cornell, CS5785-2020

Linear Regression



Slide Credit: Amuller, COMS4995

Linear Regression



Slide Credit: Amuller, COMS4995

Linear Regression

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

We will see many algorithms for this task. For now, let's call the `sklearn.linear_model` library to find a θ_1, θ_0 that fit the data well.

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Linear Regression

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In [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
```

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Linear Regression

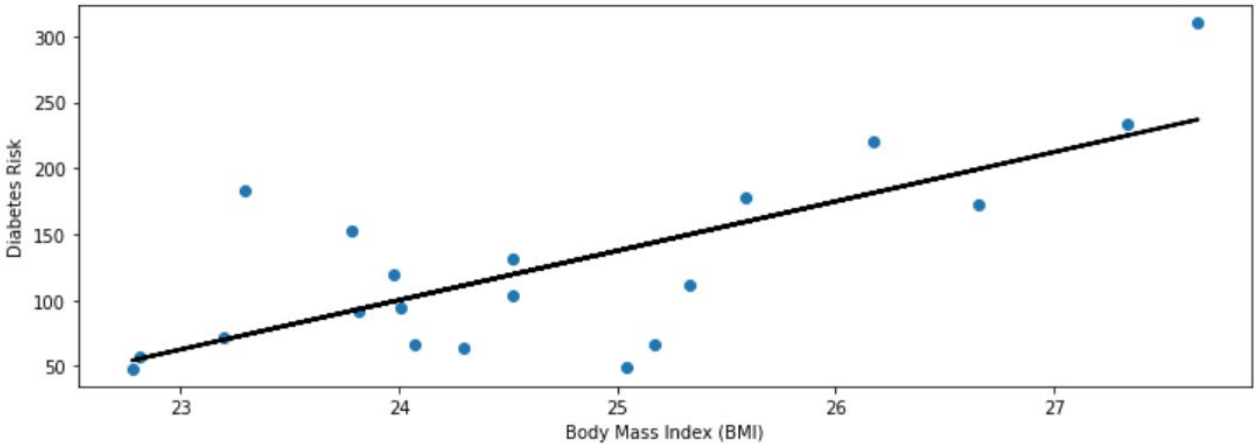
The supervised learning algorithm gave us a pair of parameters θ_1^*, θ_0^*. These define the *predictive model* f^*, defined as

$$f(x) = \theta_1^* \cdot x + \theta_0^*,$$

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

Linear Regression

```
In [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)

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



Slide Credit: Cornell, CS5785-2020

Predictions Using Supervised Learning

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

Given a new x', we can output a predicted y' as

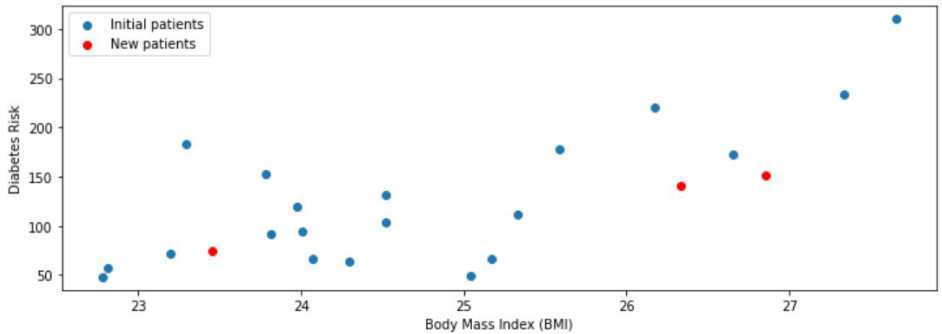
$$y' = f(x') = \theta_1^* \cdot x' + \theta_0 .$$

Slide Credit: Cornell, CS5785-2020

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

In [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'])
```

Out[8]:
```
<matplotlib.legend.Legend at 0x1259cd390>
```

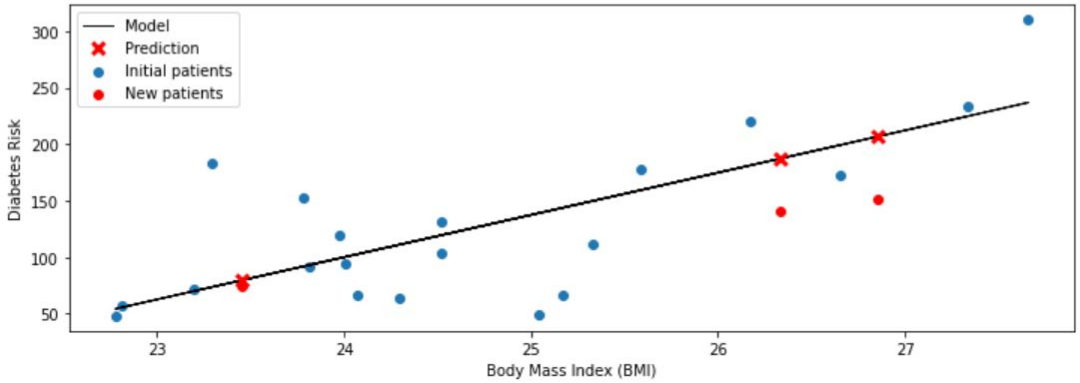


Slide Credit: Cornell, CS5785-2020

Our linear model provides an estimate of the diabetes risk for these patients.

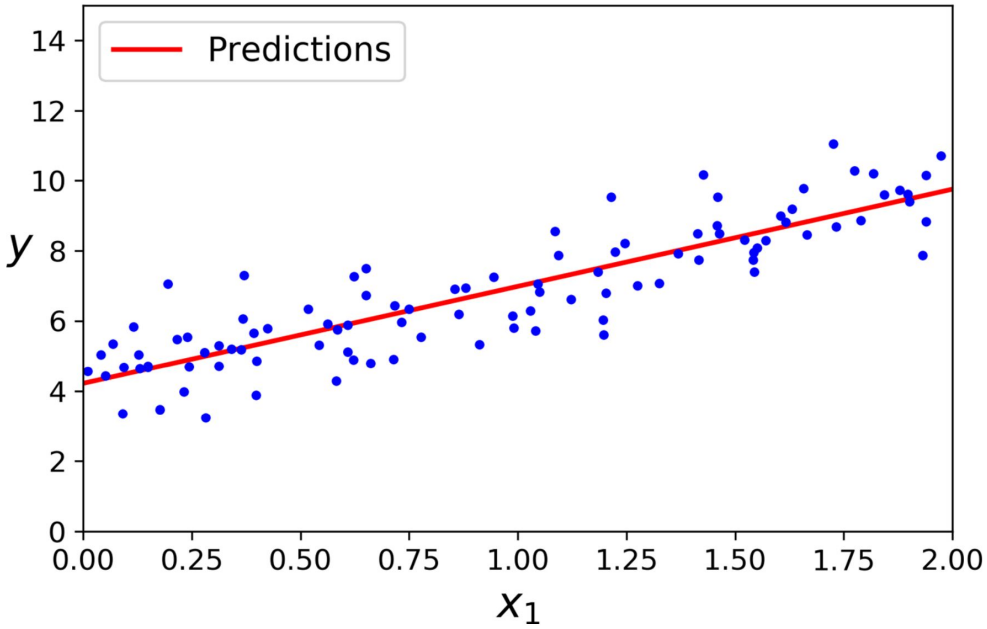
In [9]:
```
# generate predictions on the new patients
diabetes_y_test_pred = regr.predict(diabetes_X_test)

# 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, marker
size=8)
plt.legend(['Model', 'Prediction', 'Initial patients', 'New patients'])
```

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



Slide Credit: Cornell, CS5785-2020

Linear Regression



$$\hat{y} = w^T \mathbf{x} + b = \sum_{i=1}^{p} w_i x_i + b$$

Slide Credit: Amuller, COMS4995

Linear Model

Recall that a linear model has the form

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

where $x \in \mathbb{R}^d$ is a vector of features and y is the target. The θ_j are the *parameters* of the model.

By using the notation $x_0 = 1$, we can represent the model in a vectorized form

$$f_\theta(x) = \sum_{j=0}^{d} \theta_j \cdot x_j = \theta^\top x.$$

Slide Credit: Cornell, CS5785-2020

Linear Model

Let's define our model in Python.

In [26]:

```python
def f(X, theta):
    """The linear model we are trying to fit.

    Parameters:
    theta (np.array): d-dimensional vector of parameters
    X (np.array): (n,d)-dimensional data matrix

    Returns:
    y_pred (np.array): n-dimensional vector of predicted targets
    """
    return X.dot(theta)
```

Slide Credit: Cornell, CS5785-2020

An Objective: Mean Squared Error

We pick θ to minimize the mean squared error (MSE). Slight variants of this objective are also known as the residual sum of squares (RSS) or the sum of squared residuals (SSR).

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

In other words, we are looking for the best compromise in θ over all the data points.

Slide Credit: Cornell, CS5785-2020

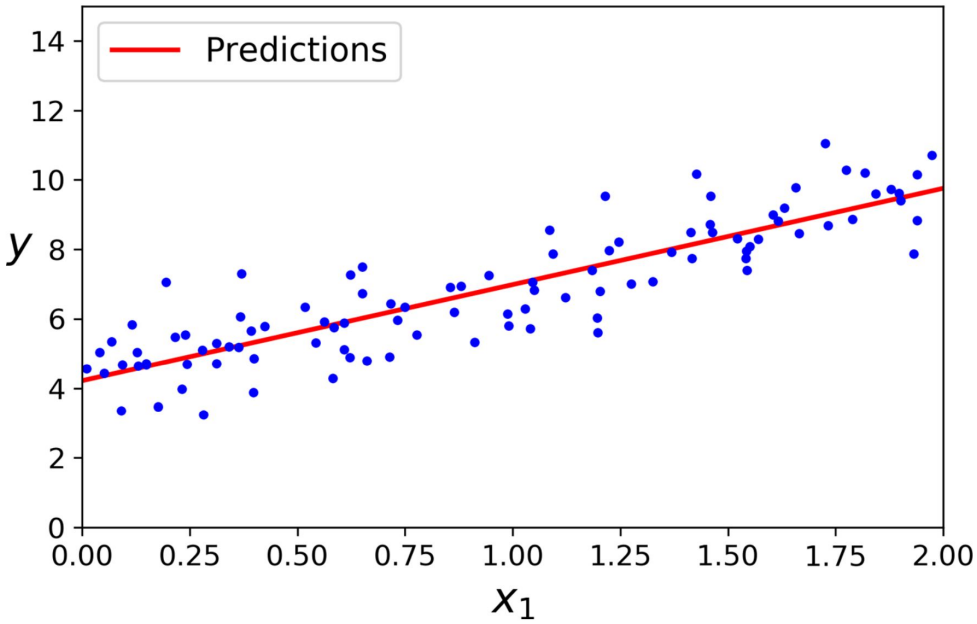
An Objective: Mean Squared Error

Let's implement mean squared error.

In [27]:
```
def mean_squared_error(theta, X, y):
    """The cost function, J, describing the goodness of fit.

    Parameters:
    theta (np.array): d-dimensional vector of parameters
    X (np.array): (n,d)-dimensional design matrix
    y (np.array): n-dimensional vector of targets
    """
    return 0.5*np.mean((y-f(X, theta))**2)
```

Slide Credit: Cornell, CS5785-2020

Linear Regression

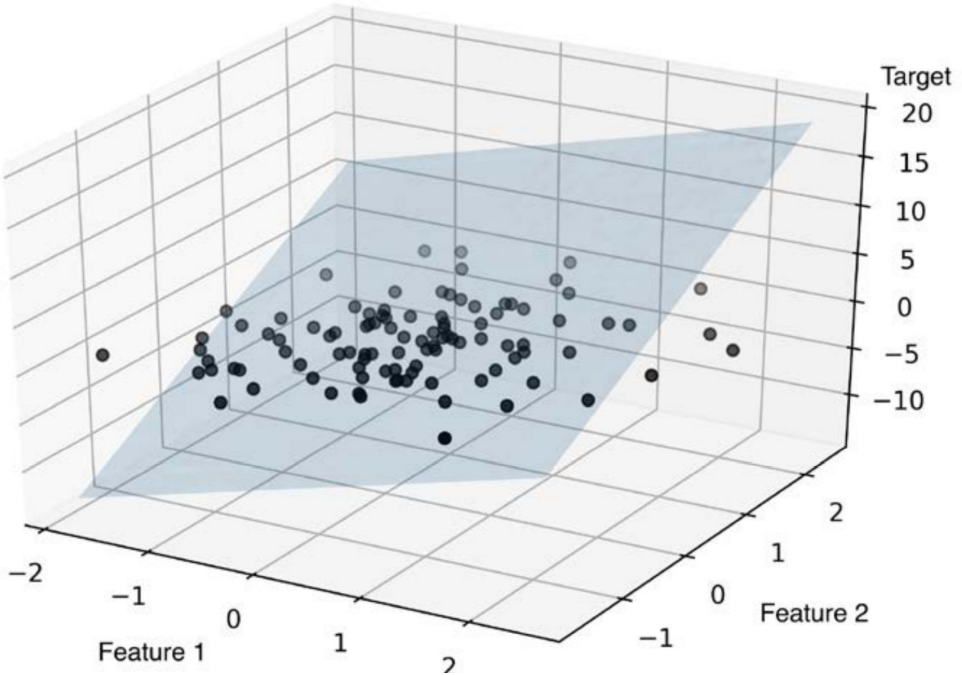


$$\hat{y} = w^T \mathbf{x} + b = \sum_{i=1}^{p} w_i x_i + b$$

$$\min_{w \in \mathbb{R}^p, b \in \mathbb{R}} \sum_{i=1}^{n} (w^T \mathbf{x}_i + b - y_i)^2$$

Slide Credit: Amuller, COMS4995

Multiple Linear Regression



$$y = w_0x_0 + w_1x_1 + \ldots + w_mx_m = \sum_{i=0}^{n} w_ix_i = w^Tx$$

Slide Credit: Rascka, Python Machine Learning

Non Linear Least Squares

So far, we have learned about a very simple linear model. These can capture only simple linear relationships in the data. How can we use what we learned so far to model more complex relationships?

We will now see a simple approach to model complex non-linear relationships called *least squares*.

Slide Credit: Cornell, CS5785-2020

Non Linear Least Squares

Recall that a polynomial of degree p is a function of the form

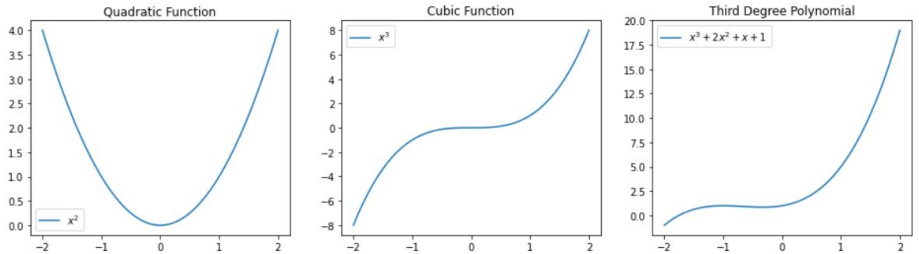
$$a_p x^p + a_{p-1} x^{p-1} + \ldots + a_1 x + a_0.$$

Below are some examples of polynomial functions.

Non Linear Least Squares

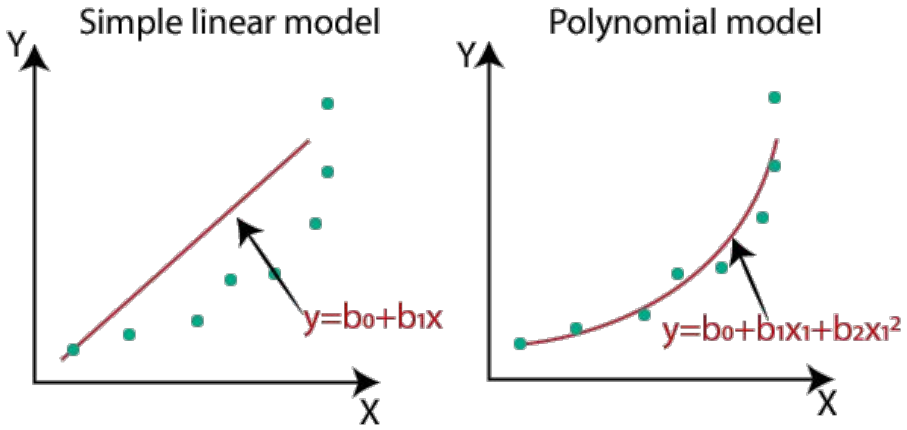
In [24]:
```
import warnings
warnings.filterwarnings("ignore")

plt.figure(figsize=(16,4))
x_vars = np.linspace(-2, 2)

plt.subplot('131')
plt.title('Quadratic Function')
plt.plot(x_vars, x_vars**2)
plt.legend(["$x^2$"])

plt.subplot('132')
plt.title('Cubic Function')
plt.plot(x_vars, x_vars**3)
plt.legend(["$x^3$"])

plt.subplot('133')
plt.title('Third Degree Polynomial')
plt.plot(x_vars, x_vars**3 + 2*x_vars**2 + x_vars + 1)
plt.legend(["$x^3 + 2 x^2 + x + 1$"])
```

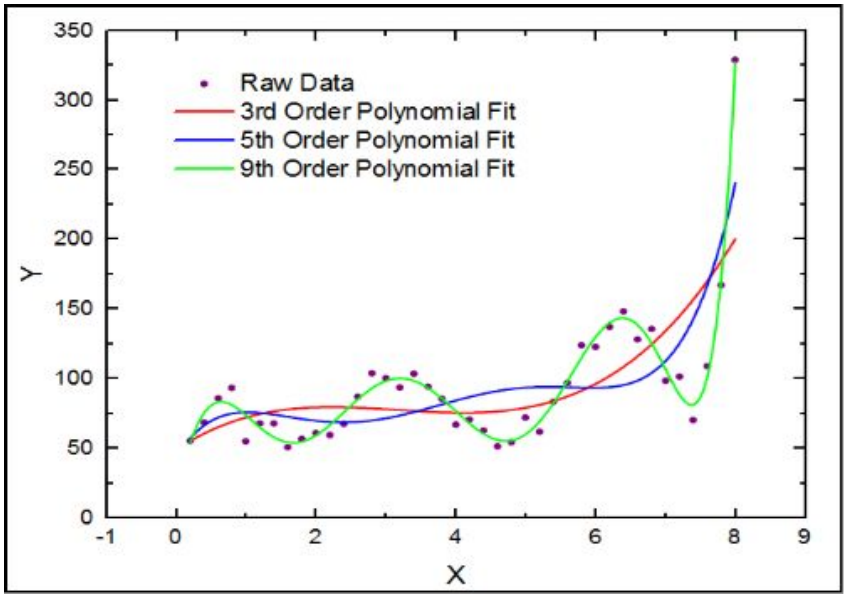
Out[24]:
```
<matplotlib.legend.Legend at 0x128ed2ac8>
```



Slide Credit: Cornell, CS5785-2

Polynomial Regression





Non Linear Least Squares

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```
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plt.plot(x_vars, x_vars**3)
plt.legend(["$x^3$"])

plt.subplot('133')
plt.title('Third Degree Polynomial')
plt.plot(x_vars, x_vars**3 + 2*x_vars**2 + x_vars + 1)
plt.legend(["$x^3 + 2 x^2 + x + 1$"])
```
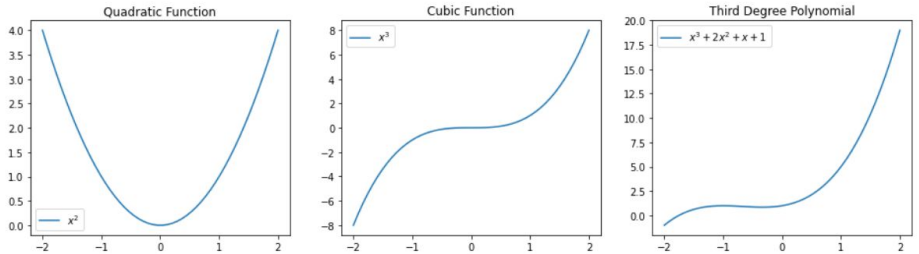

Out[24]:
```
<matplotlib.legend.Legend at 0x128ed2ac8>
```



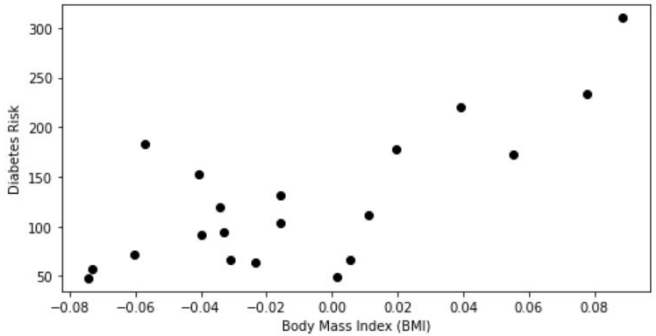
Slide Credit: Cornell, CS5785-2

In [25]:

```
%matplotlib inline
import matplotlib.pyplot as plt
plt.rcParams['figure.figsize'] = [8, 4]

import numpy as np
import pandas as pd
from sklearn import datasets

# Load the diabetes dataset
X, y = datasets.load_diabetes(return_X_y=True, as_frame=True)

# add an extra column of onens
X['one'] = 1

# Collect 20 data points
X_train = X.iloc[-20:]
y_train = y.iloc[-20:]

plt.scatter(X_train.loc[:,['bmi']], y_train,  color='black')
plt.xlabel('Body Mass Index (BMI)')
plt.ylabel('Diabetes Risk')
```

Out[25]:

```
Text(0, 0.5, 'Diabetes Risk')
```



Diabetes Dataset: A Non-Linear Featurization

Let's now obtain linear features for this dataset.

In [26]:
```
X_bmi = X_train.loc[:, ['bmi']]

X_bmi_p3 = pd.concat([X_bmi, X_bmi**2, X_bmi**3], axis=1)
X_bmi_p3.columns = ['bmi', 'bmi2', 'bmi3']
X_bmi_p3['one'] = 1
X_bmi_p3.head()
```

Out[26]:

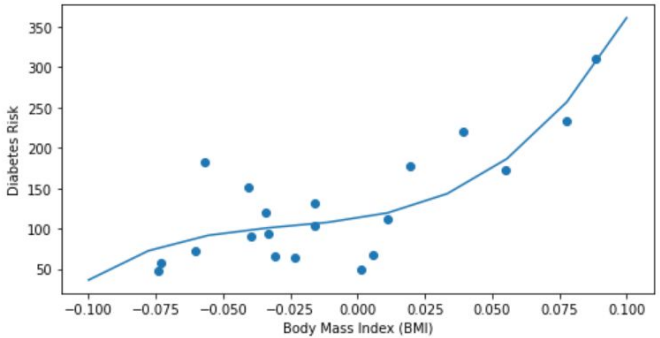
	bmi	bmi2	bmi3	one
422	0.077863	0.006063	0.000472	1
423	-0.039618	0.001570	-0.000062	1
424	0.011039	0.000122	0.000001	1
425	-0.040696	0.001656	-0.000067	1
426	-0.034229	0.001172	-0.000040	1

Slide Credit: Cornell, CS5785-2020

Dia ion

In [27]:
```
# Fit a linear regression
theta = np.linalg.inv(X_bmi_p3.T.dot(X_bmi_p3)).dot(X_bmi_p3.T).dot(y_train)

# Show the learned polynomial curve
x_line = np.linspace(-0.1, 0.1, 10)
x_line_p3 = np.stack([x_line, x_line**2, x_line**3, np.ones(10,)], axis=1)
y_train_pred = x_line_p3.dot(theta)

plt.xlabel('Body Mass Index (BMI)')
plt.ylabel('Diabetes Risk')
plt.scatter(X_bmi, y_train)
plt.plot(x_line, y_train_pred)
```

Out[27]:
```
[<matplotlib.lines.Line2D at 0x1292c99e8>]
```



Slide Credit: Cornell, CS5785-2020

Evaluation Metrics

- Pearson correlation
- R-squared, or R^2
- Adjusted- R-squared
- Mean Squared Error
- Mean Absolute Error
- Root Mean Squared Error

Pearson Correlation

- *Pearson's r*
- Is a measure of linear correlation between two sets of data.
- It is the ratio between the *covariance* of two variables and the product of their *standard deviations.*
- The results always has a value between -1 and 1.

$$r = \frac{\sum (x_i - \bar{x})(y_i - \bar{y})}{\sqrt{\sum (x_i - \bar{x})^2 \sum (y_i - \bar{y})^2}}$$

Where,

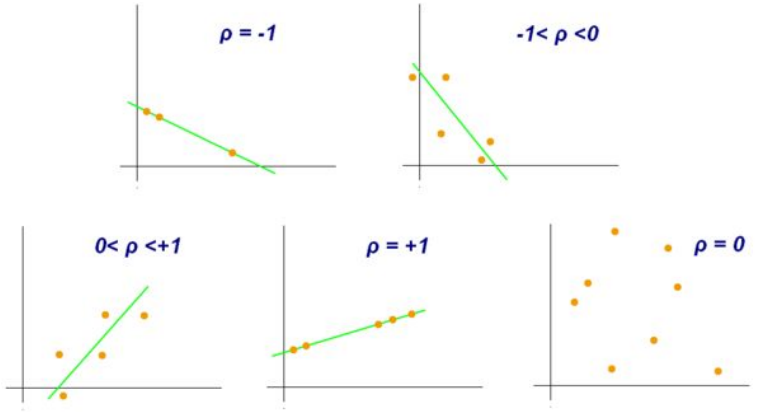
r = Pearson Correlation Coefficient

x_i = x variable samples

y_i = y variable sample

$\bar{x}$ = mean of values in x variable

$\bar{y}$ =mean of values in y variable



Slide Credit: https://en.wikipedia.org/wiki/Pearson_correlation_coefficient

Coefficient of Determination

- R-squared, or R^2
- R-squared ranges from 0 to 1 and measures the proportion of variation in the data that is accounted for in the model.
- It is useful mainly in explanatory uses of regression where you want to assess how well the model fits the data.
- **Note**: It does not take into consideration of overfitting problem. If your model has many independent variables, due to model is too complicated, it may fit very well to the training data but performs badly for testing data.

$$R^2 = 1 - \frac{\sum_{i=1}^{n} (y_i - \hat{y}_i)^2}{\sum_{i=1}^{n} (y_i - \bar{y})^2}$$

Slide Credit: Peter Bruce, Practical Statistics for Data Scientist

Adjusted R^2

- The disadvantage of the R_square score is while adding new features in data the R_square score starts increasing or remains constant but never decreases because it assumes that while adding more data variance of data increases.

$$Adjusted\ R^2 = 1 - \frac{(1 - R^2)(N - 1)}{N - p - 1}$$

Where

R^2 Sample R-Squared

N Total Sample Size

p Number of independent variable

- Where where n is the total number of observations and p is the number of predictors. Adjusted R^2 will always be less than or equal to R^2.

Slide Credit: Peter Bruce, Practical Statistics for Data Scientist

Adjusted R^2

Case 1		Case 2			Case 3		
Var1	Y	Var1	Var2	Y	Var1	Var2	Y
x1	y1	x1	2*x1	y1	x1	2*x1+0.1	y1
x2	y2	x2	2*x2	y2	x2	2*x2	y2
x3	y3	x3	2*x3	y3	x3	2*x3 + 0.1	y3
x4	y4	x4	2*x4	y4	x4	2*x4	y4
x5	y5	x5	2*x5	y5	x5	2*x5 + 0.1	y5

	Case 1	Case 2	Case 3
R_squared	0.985	0.985	0.987
Adj_R_squared	0.981	0.971	0.975

Slide Credit: https://medium.com/usf-msds/choosing-the-right-metric-for-machine-learning-models-part-1-a99d7d7414e4

Mean Square Error (MSE)

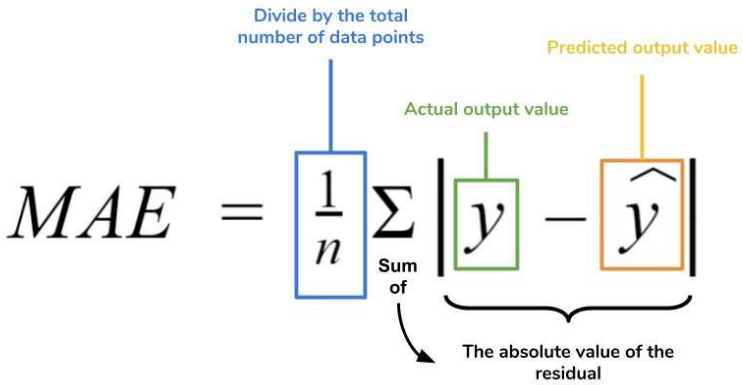
- MSE is calculated by the sum of square of prediction error which is real output minus predicted output and the divide by the number of data points.
- It is hard to interpret many insights from one single result but it gives you a real number to compare against other model results and help you select the best regression model.
- If you have outliers in the dataset then it penalizes the outliers most and the calculated MSE is bigger (-).

$$MSE = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

Slide Credit: Songhao Wu

Mean Absolute Error (MAE)

- Same unit as the output variable (+)
- Robust to outliers (+)



Slide Credit: Songhao Wu

Root Mean Square Error (MSE)

$$RMSE = \sqrt{\sum_{i=1}^{n} \frac{(\hat{y}_i - y_i)^2}{n}}$$

Choosing the right metric

- A nice blog post that you can read more about metrics for evaluation regression models.
  - https://medium.com/usf-msds/choosing-the-right-metric-for-machine-learning-models-part-1-a99d7d7414e4

Case 1: Actual Values = [2,4,6,8] , Predicted Values = [4,6,8,10]

Case 2: Actual Values = [2,4,6,8] , Predicted Values = [4,6,8,12]

MAE for case 1 = 2.0, RMSE for case 1 = 2.0

MAE for case 2 = 2.5, RMSE for case 2 = 2.65

Slide Credit: Songhao Wu

Calculus Review: Derivatives

Recall that the derivative

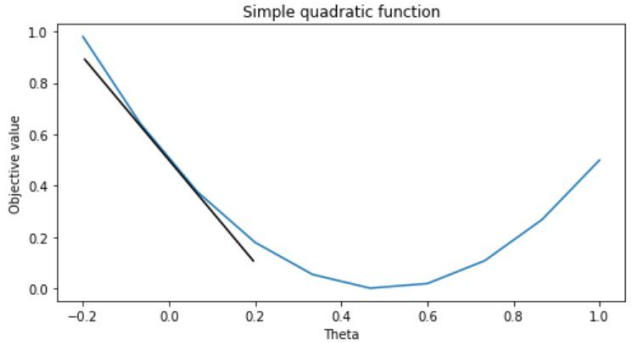
$$\frac{df(\theta_0)}{d\theta}$$

of a univariate function $f : \mathbb{R} \to \mathbb{R}$ is the instantaneous rate of change of the function $f(\theta)$ with respect to its parameter θ at the point θ_0.

Calculus Review: Derivatives

In [5]:
```
def quadratic_derivative(theta):
    return (2*theta-1)*2

df0 = quadratic_derivative(np.array([[0]])) # derivative at zero
f0 = quadratic_function(np.array([[0]]))
line_length = 0.2

plt.plot(thetas, f_vals)
plt.annotate('', xytext=(0-line_length, f0-line_length*df0), xy=(0+line_length,
f0+line_length*df0),
             arrowprops={'arrowstyle': '-', 'lw': 1.5}, va='center', ha='cente
r')
plt.xlabel('Theta')
plt.ylabel('Objective value')
plt.title('Simple quadratic function')
```

Out[5]:
```
Text(0.5, 1.0, 'Simple quadratic function')
```



Calculus Review: Partial Derivatives

The partial derivative

$$\frac{\partial f(\theta_0)}{\partial \theta_j}$$

of a multivariate function $f : \mathbb{R}^d \to \mathbb{R}$ is the derivative of f with respect to θ_j while all othe other inputs θ_k for $k \neq j$ are fixed.

Slide Credit: Cornell Cs 5785

Calculus Review: The Gradient

The gradient $\nabla_\theta f$ further extends the derivative to multivariate functions $f : \mathbb{R}^d \to \mathbb{R}$, and is defined at a point θ_0 as

$$\nabla_\theta f(\theta_0) = \begin{bmatrix} \frac{\partial f(\theta_0)}{\partial \theta_1} \\ \frac{\partial f(\theta_0)}{\partial \theta_2} \\ \vdots \\ \frac{\partial f(\theta_0)}{\partial \theta_d} \end{bmatrix}.$$

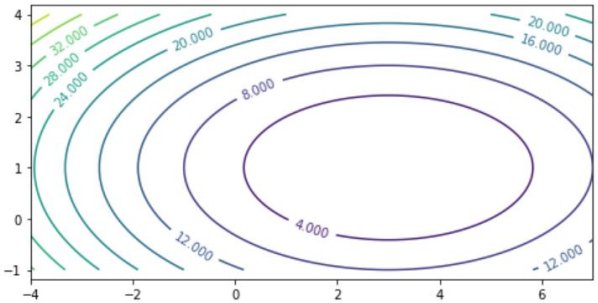
The j-th entry of the vector $\nabla_\theta f(\theta_0)$ is the partial derivative $\frac{\partial f(\theta_0)}{\partial \theta_j}$ of f with respect to the j-th component of θ.

Calculus Review: The Gradient

Let's visualize this function.

In [8]:
```
theta0_grid = np.linspace(-4,7,101)
theta1_grid = np.linspace(-1,4,101)
theta_grid = theta0_grid[np.newaxis,:], theta1_grid[:,np.newaxis]
J_grid = quadratic_function2d(theta0_grid[np.newaxis,:], theta1_grid[:,np.newax
is])

X, Y = np.meshgrid(theta0_grid, theta1_grid)
contours = plt.contour(X, Y, J_grid, 10)
plt.clabel(contours)
plt.axis('equal')
```

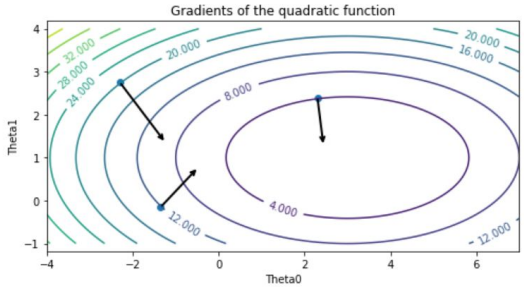
Out[8]: (-4.0, 7.0, -1.0, 4.0)



Calculus Review: The Gradient

In [10]:
```
theta0_pts, theta1_pts = np.array([2.3, -1.35, -2.3]), np.array([2.4, -0.15, 2.
75])
dfs = quadratic_derivative2d(theta0_pts, theta1_pts)
line_length = 0.2

contours = plt.contour(X, Y, J_grid, 10)
for theta0_pt, theta1_pt, df0 in zip(theta0_pts, theta1_pts, dfs):
    plt.annotate('', xytext=(theta0_pt, theta1_pt),
                     xy=(theta0_pt-line_length*df0[0], theta1_pt-line_length*df
0[1]),
                     arrowprops={'arrowstyle': '->', 'lw': 2}, va='center', ha
='center')
plt.scatter(theta0_pts, theta1_pts)
plt.clabel(contours)
plt.xlabel('Theta0')
plt.ylabel('Theta1')
plt.title('Gradients of the quadratic function')
plt.axis('equal')
```

Out[10]: (-4.0, 7.0, -1.0, 4.0)



Slide Credit: Cornell Cs 5785

Gradient Descent

Gradient descent is a very common optimization algorithm used in machine learning.

The intuition behind gradient descent is to repeatedly obtain the gradient to determine the direction in which the function decreases most steeply and take a step in that direction.

Slide Credit: Cornell CS 5785

Gradient Descent: Notation

More formally, if we want to optimize $J(\theta)$, we start with an initial guess θ_0 for the parameters and repeat the following update until θ is no longer changing:

$$\theta_i := \theta_{i-1} - \alpha \cdot \nabla_\theta J(\theta_{i-1}).$$

As code, this method may look as follows:

```
theta, theta_prev = random_initialization()
while norm(theta - theta_prev) > convergence_threshold:
    theta_prev = theta
    theta = theta_prev - step_size * gradient(theta_prev)
```

In the above algorithm, we stop when $||\theta_i - \theta_{i-1}||$ is small.

Slide Credit: Cornell CS 5785

Mean Squared Error: Partial Derivatives

Let's work out what a partial derivative is for the MSE error loss for a linear model.

$$
\begin{aligned}
\frac{\partial J(\theta)}{\partial \theta_j} &= \frac{\partial}{\partial \theta_j} \frac{1}{2} (f_\theta(x) - y)^2 \\
&= (f_\theta(x) - y) \cdot \frac{\partial}{\partial \theta_j} (f_\theta(x) - y) \\
&= (f_\theta(x) - y) \cdot \frac{\partial}{\partial \theta_j} \left(\sum_{k=0}^{d} \theta_k \cdot x_k - y \right) \\
&= (f_\theta(x) - y) \cdot x_j
\end{aligned}
$$

Slide Credit: Cornell CS 5785

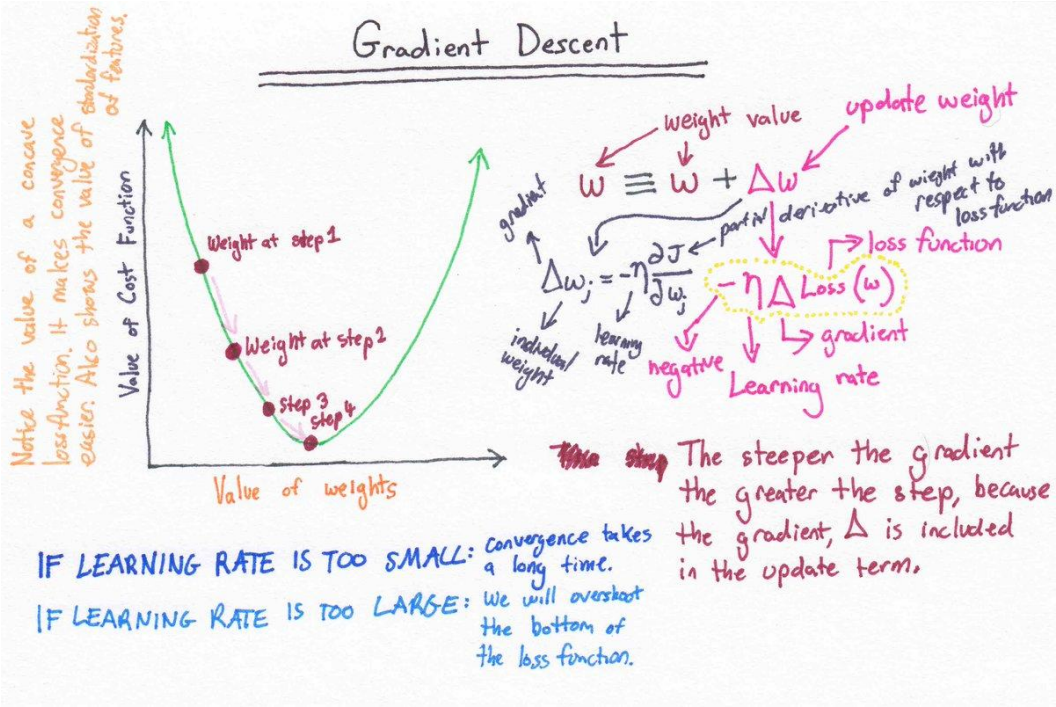
Mean Squared Error: Partial Derivatives

Let's implement the gradient.

In [28]:
```python
def mse_gradient(theta, X, y):
    """The gradient of the cost function.

    Parameters:
    theta (np.array): d-dimensional vector of parameters
    X (np.array): (n,d)-dimensional design matrix
    y (np.array): n-dimensional vector of targets

    Returns:
    grad (np.array): d-dimensional gradient of the MSE
    """
    return np.mean((f(X, theta) - y) * X.T, axis=1)
```

Slide Credit: Cornell CS 5785

Gradient Descent

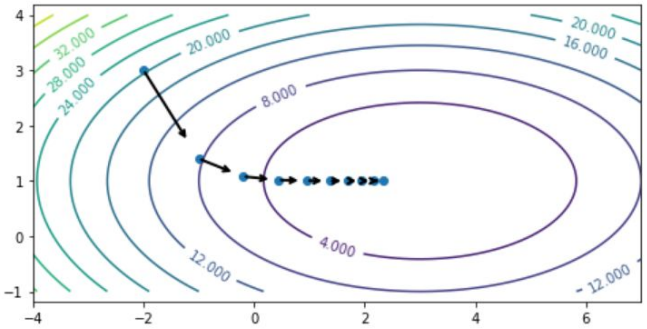


Slide Credit: Machine Learning Flashcards

We can now visualize gradient descent.

In [25]:
```
opt_pts = np.array(opt_pts)
opt_grads = np.array(opt_grads)

contours = plt.contour(X, Y, J_grid, 10)
plt.clabel(contours)
plt.scatter(opt_pts[:,0], opt_pts[:,1])

for opt_pt, opt_grad in zip(opt_pts, opt_grads):
    plt.annotate('', xytext=(opt_pt[0], opt_pt[1]),
                 xy=(opt_pt[0]-0.8*step_size*opt_grad[0], opt_pt[1]-0.8*step_si
ze*opt_grad[1]),
                 arrowprops={'arrowstyle': '->', 'lw': 2}, va='center', ha='cen
ter')

plt.axis('equal')
```

Out[25]:
```
(-4.0, 7.0, -1.0, 4.0)
```



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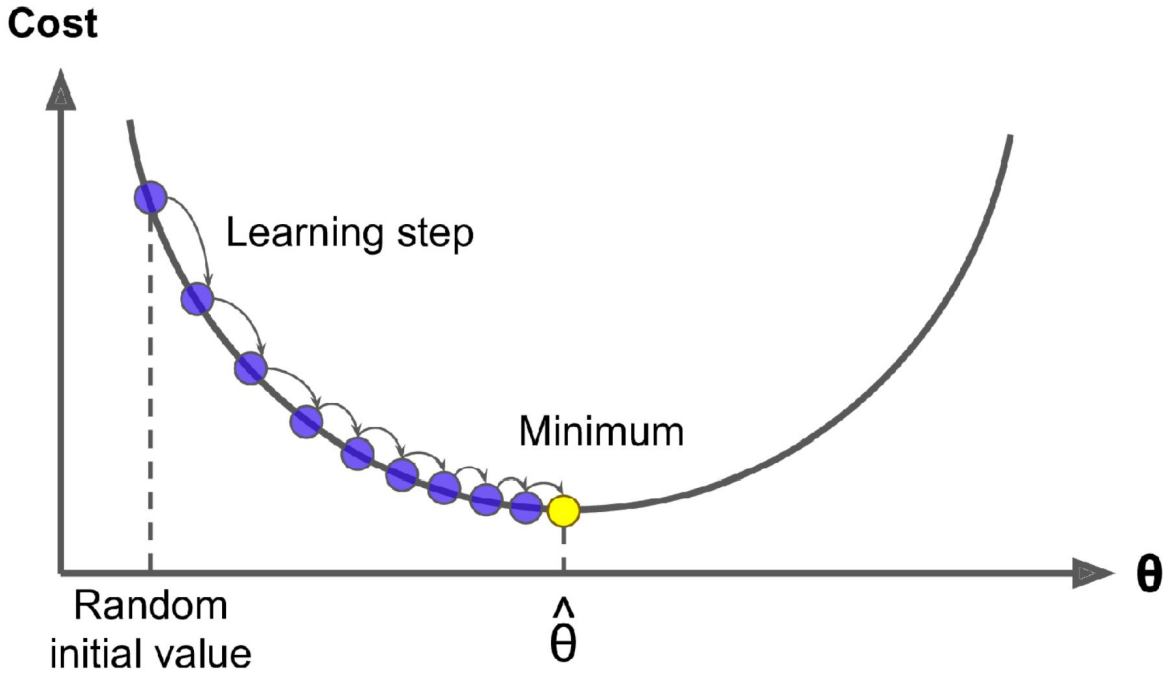
Gradient Descent



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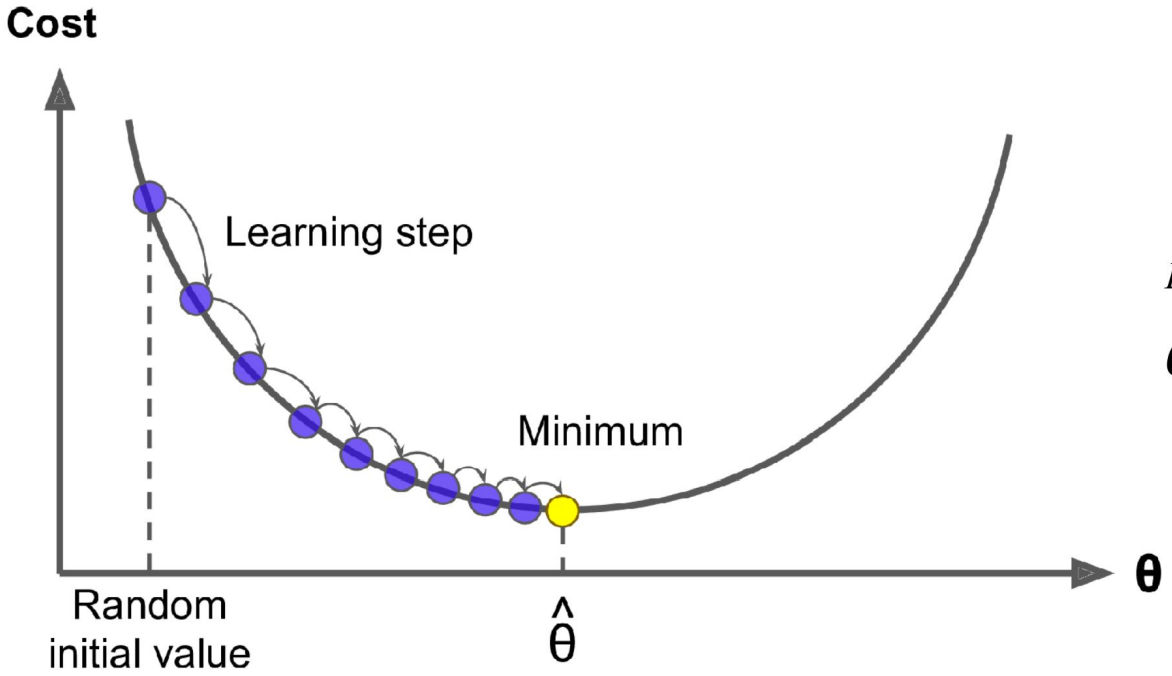
Gradient Descent



Equation 4-7. Gradient Descent step

$$\boldsymbol{\theta}^{(\text{next step})} = \boldsymbol{\theta} - \eta \nabla_{\boldsymbol{\theta}} \operatorname{MSE}(\boldsymbol{\theta})$$

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Gradient Descent

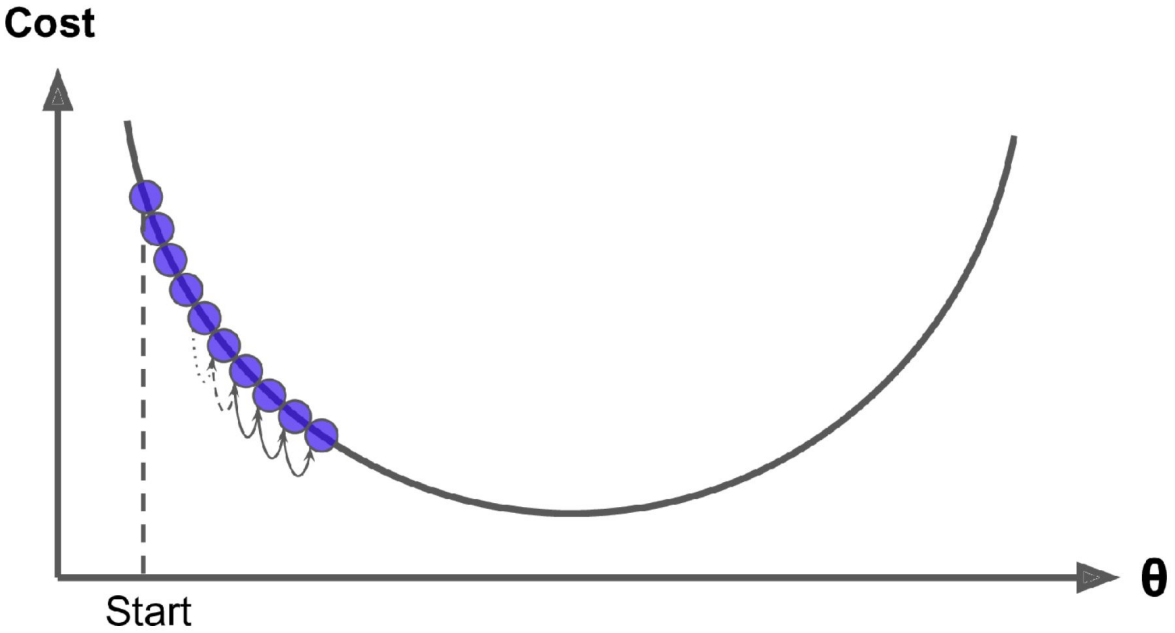

Figure 4-4. The learning rate is too small

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Gradient Descent

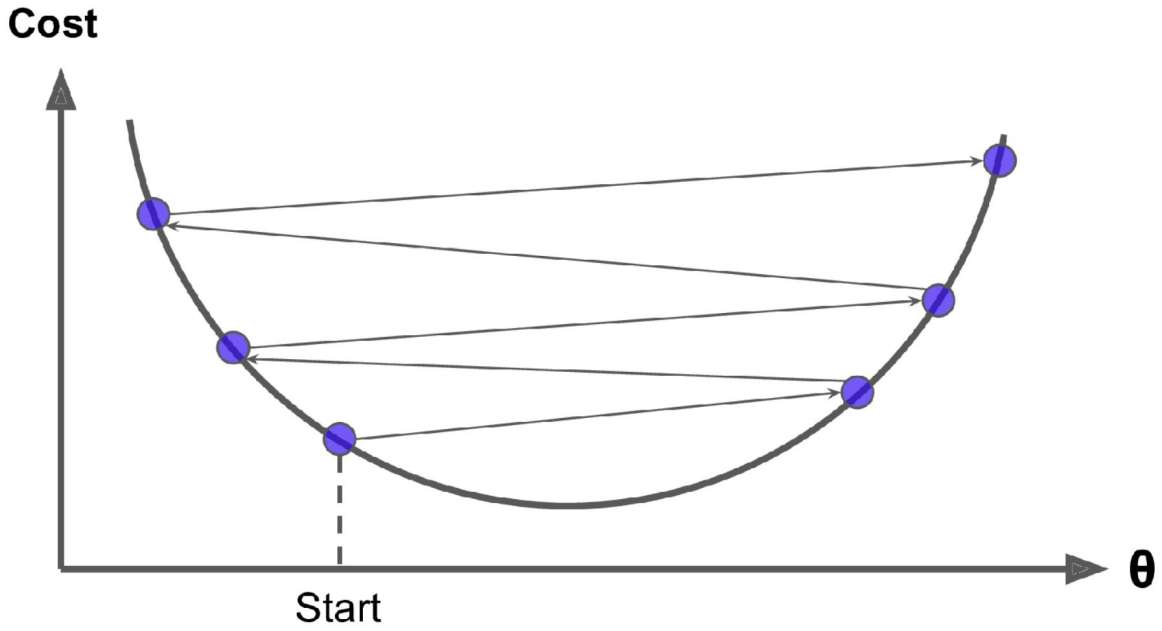

Figure 4-5. The learning rate is too large

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Gradient Descent

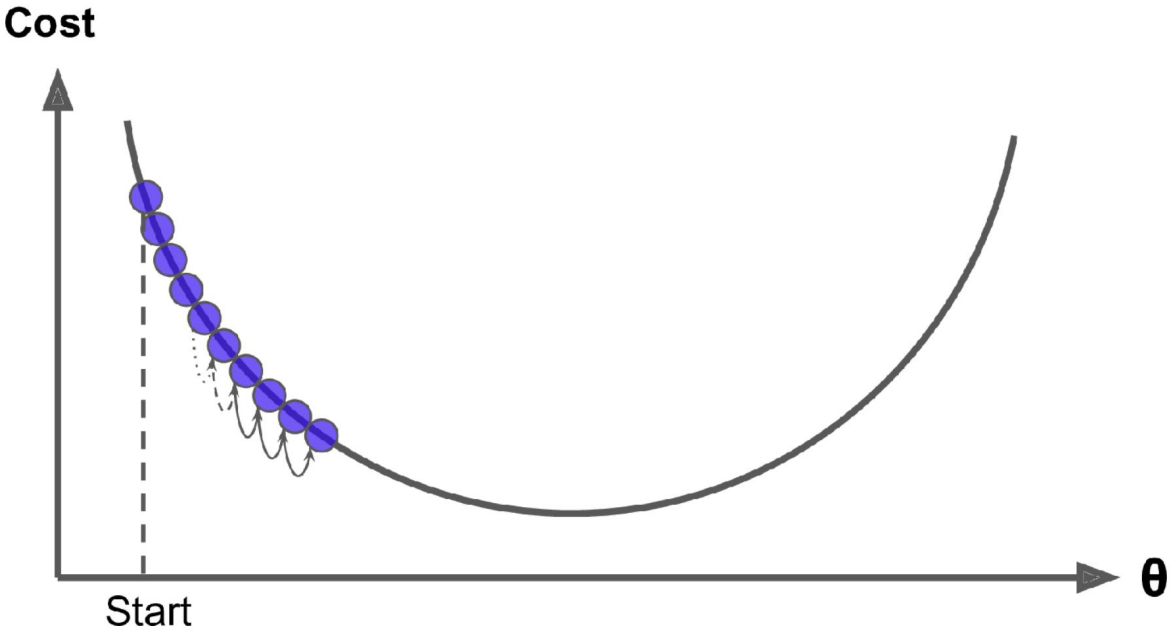

Figure 4-4. The learning rate is too small

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Gradient Descent

- Check this blog post for interactive explanation of Linear Regression
  - https://machinelearningcompass.com/machine_learning_math/gradient_descent_for_linear_regression/

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