Data Analysis 2025

Chapter IV: Linear Regression

Learning Goals

- Formulate learning problems using appropriate loss functions
- Indicate ways of finding the optimal parameters of a model
- Develop & experiment linear regression models (simple and multiple)
- Assess the fit of regression models in different ways
- Diagnose a bad fit in different ways
- Determine proper transformations for variables in modelling (e.g. linearization, categorical variables)
- Explain the concepts of over/under-fitting and the bias/variance trade-off
- Assess when a model is leaning towards overfitting
- Apply cross-validation (CV) (and K-fold CV) to your models
- Explain concepts like data leakage

Announcements

- Clinic 1 is due this Friday (late night). Wildcards are available and they apply to the whole group.
- If you still don't have a group, use Discord to self-organize
- The "wildcards standout dilemma" : If you keep the same group for all clinics, then things are easy. If you change groups per clinic, then things become tricky.
  - e.g. if your groups submits clinic 1 3 days late, then each of the group members uses 3 wildcards (fair and square). If for clinic 2 there is a different composition with different wildcard balances among team members and in order to avoid system misuse, the group remaining wildcard balance will be computed the minimum of wildcards available (i.e. if 1 members has used 4 wildcards and 2 members have used 2 wildcards, then the group has an overall balance of 2 wildcards left).
- Quizz 1 is avalable, Bootcamp 1 solution will be available shortly
- Bootcamps are graded on participation and are meant to be (mostly) completed in class

Components of a Supervised Machine Learning Problem

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

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

of the Objective Fct

Loss

We have Inputs x and outp

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

Supervised Learning: Notations and Basics

the target label

A Supervised Learning Dataset: Notation

"i" is the Data Point

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

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

Input

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*.

Training Dataset: Inputs

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

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

d different Features

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, $\mathcal{X} = \mathbb{R}^d$. Feature Space

We refer to the variables describing the patient as *attributes*. Examples of attributes include:

Original from the Data

- The age of a patient.
- The patient's gender.
- The patient's BMI.

Features: When I do Transform

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*, however in practice sometimes the terms are used interchangeably.

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.

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 $J(\theta) : \Theta \to [0, \infty)$.

Error-based objective functions for regression are typically lower-bounded by 0, but in general may take any real value (e.g., for classification)

Objective: Examples

Regression

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

- Mean squared error:

L2 loss

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

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

Optimizer: Example

We will see that behind the scenes, the `sklearn.linear_models.LinearRegression` algorithm optimizes the MSE loss. When $\mathcal{X} = \mathbb{R}$, $\Theta = \mathbb{R}^2$ for the intercept and slop terms.

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

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

Part 1: Calculus Review

Before we present our first supervised learning algorithm, we will do a quick calculus review.

In class we will only discuss the basics of gradient descent but feel free to browse through the rest for a reminder.

Motivation: Optimization in ML

θ Vektor

A machine learning algorithm typically minimizes a loss function J, e.g.,:

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

transponierter Faktor

F Datenpkt

The optimizer outputs parameters θ that best "fit" the training dataset $\mathcal{D} = \{(x^{(i)}, y^{(i)}) \mid i = 1, 2, \ldots, n\}$.

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

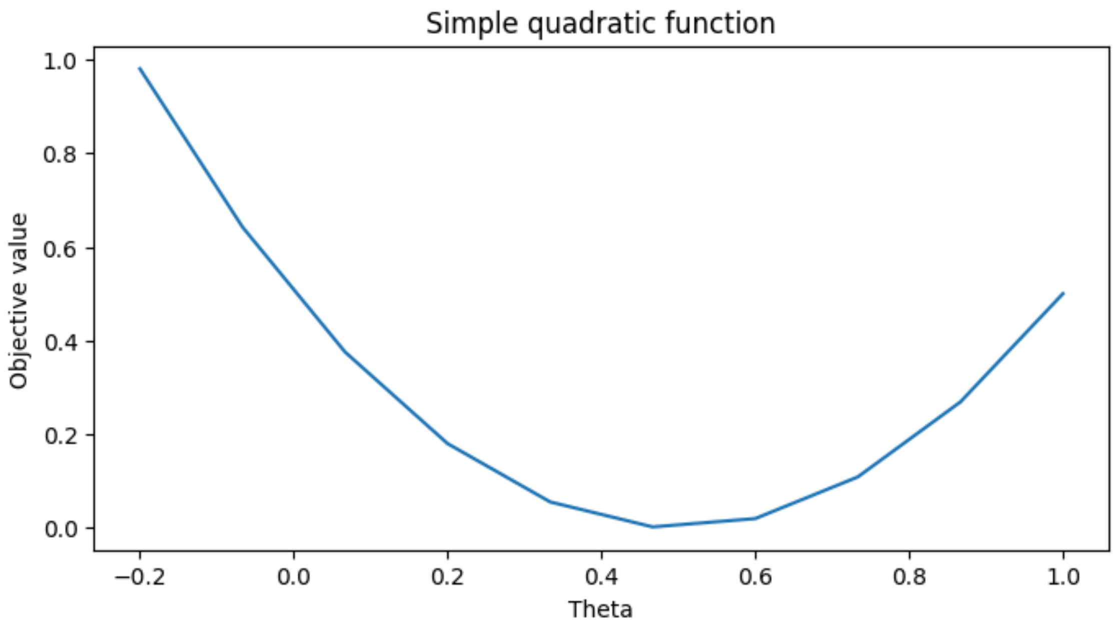
In [60]:
```
import numpy as np
import matplotlib.pyplot as plt
plt.rcParams['figure.figsize'] = [8, 4]
import seaborn as sns

import plotly.io as pio
import plotly.express as px
import plotly.graph_objects as go
pio.renderers.default = "iframe"
pio.templates["plotly"].layout.colorway = px.colors.qualitative.Vivi
px.defaults.width = 800
```

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

We can visualize it.

In [3]:
```python
# First construct a grid of theta1 parameter pairs and their corresp
# 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[3]:
```
Text(0.5, 1.0, 'Simple quadratic function')
```



Calculus Review: Derivatives

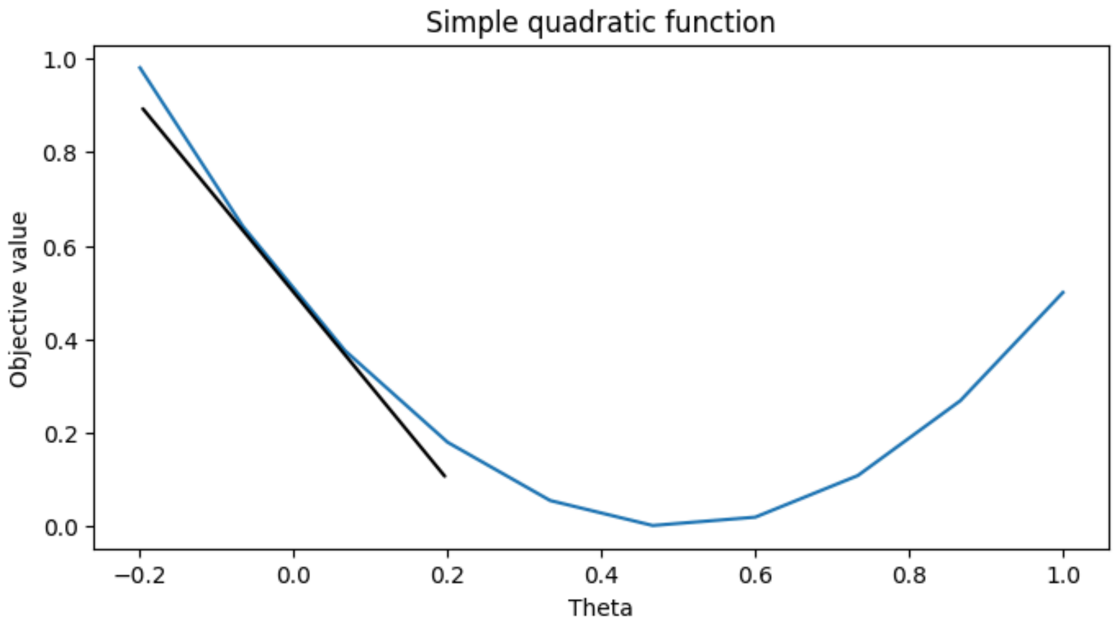
Recall that the derivative

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

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.

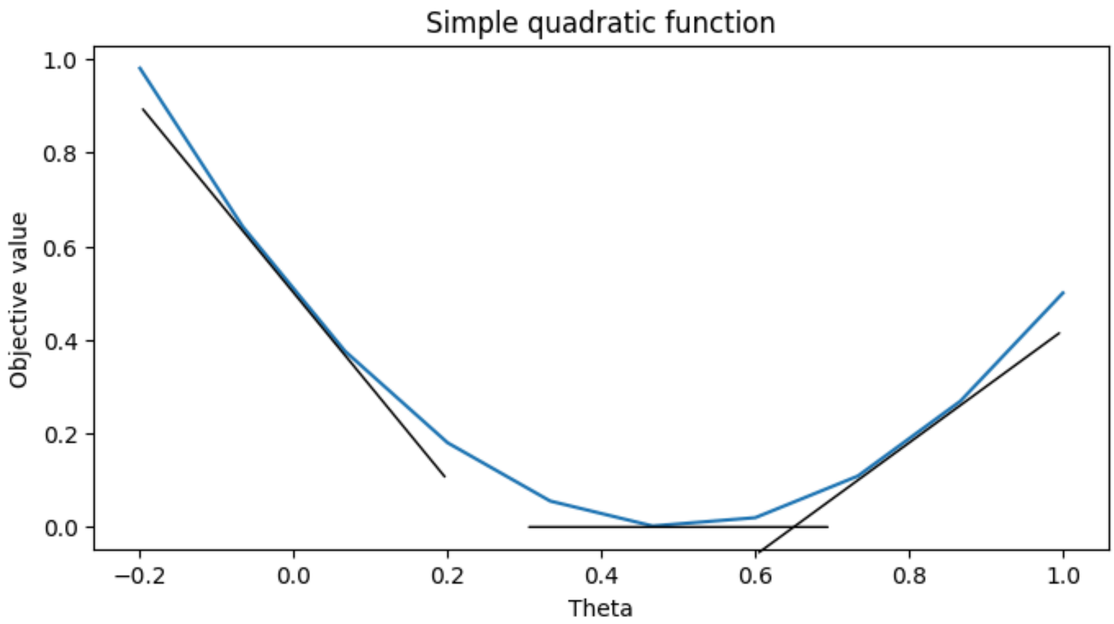
In [4]:
```python
def quadratic_derivative(theta):
    return (2*theta-1)*2

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+l
             arrowprops={'arrowstyle': '-', 'lw': 1.5}, va='center',
plt.xlabel('Theta')
plt.ylabel('Objective value')
plt.title('Simple quadratic function')
```

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



In [5]:
```
pts = np.array([[0, 0.5, 0.8]]).reshape((3,1))
df0s = quadratic_derivative(pts)
f0s = quadratic_function(pts)

plt.plot(thetas, f_vals)
for pt, f0, df0 in zip(pts.flatten(), f0s.flatten(), df0s.flatten())
    plt.annotate('', xytext=(pt-line_length, f0-line_length*df0), xy
                 arrowprops={'arrowstyle': '-', 'lw': 1}, va='center', h
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

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

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

Calculus Review: The Gradient

The gradient ∇f is the vector of all the partial derivatives:

d Parameter
↓
Partial Derivative
With Respect to every Parameter

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

Multiple Variable
(Attribute)

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

We will use a quadratic function as a running example.

$$f(\theta_0, \theta_1) = \frac{1}{2}\left((2\theta_1 - 2)^2 + (\theta_0 - 3)^2\right)$$

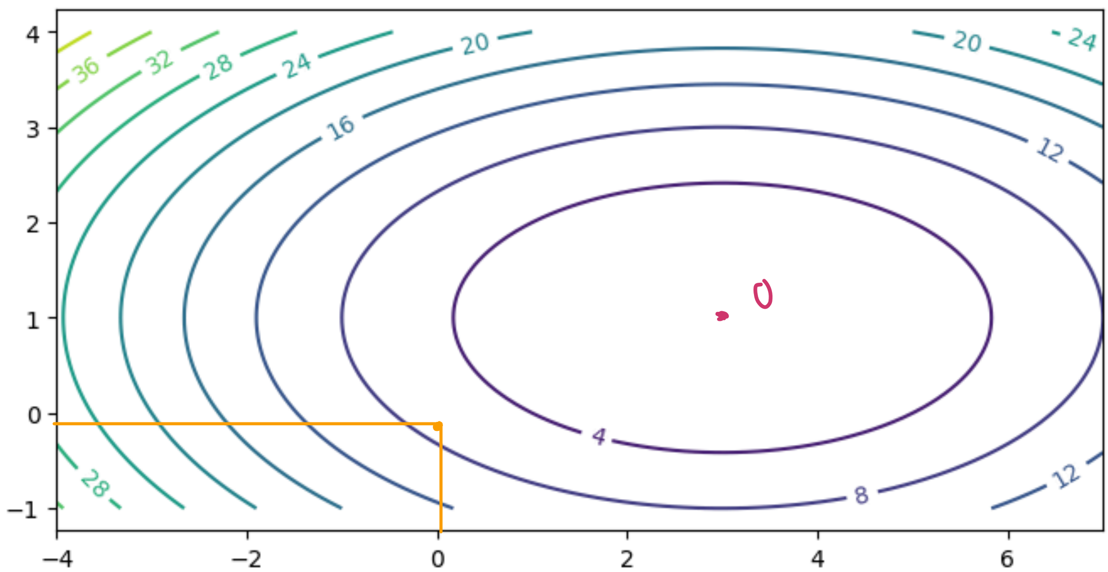
In [94]:
```
def quadratic_function2d(theta0, theta1):
    """Quadratic objective function, J(theta0, theta1).

    The inputs theta0, theta1 are 2d arrays and we evaluate
    the objective at each value theta0[i,j], theta1[i,j].
    We implement it this way so it's easier to plot the
    level curves of the function in 2d.

    Parameters:
    theta0 (np.array): 2d array of first parameter theta0
    theta1 (np.array): 2d array of second parameter theta1

    Returns:
    fvals (np.array): 2d array of objective function values
        fvals is the same dimension as theta0 and theta1.
        fvals[i,j] is the value at theta0[i,j] and theta1[i,j].
    """
    theta0 = np.atleast_2d(np.asarray(theta0))
    theta1 = np.atleast_2d(np.asarray(theta1))
    return 0.5*((2*theta1-2)**2 + (theta0-3)**2)
```

Let's visualize this function.

In [95]:
```python
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_gric

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

Level Plots

Out[95]: (-4.0, 7.0, -1.0, 4.0)



Let's write down the gradient of the ~~quadratic function.~~

$$\nabla f(\theta_0, \theta_1) = [\theta_0 - 3, (2\theta_1 - 2) \times 2]$$

In [96]:
```python
def quadratic_derivative2d(theta0, theta1):
    """Derivative of quadratic objective function.

    The inputs theta0, theta1 are 1d arrays and we evaluate
    the derivative at each value theta0[i], theta1[i].

    Parameters:
    theta0 (np.array): 1d array of first parameter theta0
    theta1 (np.array): 1d array of second parameter theta1

    Returns:
    grads (np.array): 2d array of partial derivatives
        grads is of the same size as theta0 and theta1
        along first dimension and of size
        two along the second dimension.
        grads[i,j] is the j-th partial derivative
        at input theta0[i], theta1[i].
    """
    # this is the gradient of 0.5*((2*theta1-2)**2 + (theta0-3)**2)
    grads = np.stack([theta0-3, (2*theta1-2)*2], axis=1)
    grads = grads.reshape([len(theta0), 2])
    return grads
```

We can visualize the gradient.

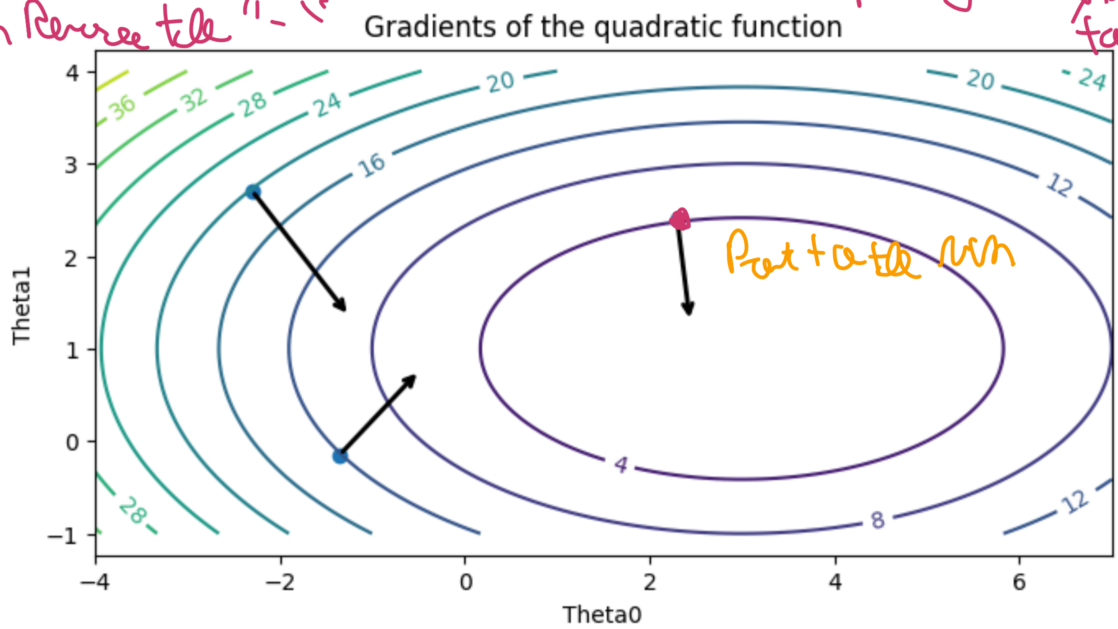
```python
theta0_pts, theta1_pts = np.array([2.3, -1.35, -2.3]), np.array([2.4
dfs = quadratic_derivative2d(theta0_pts, theta1_pts)
line_length = 0.2

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-lir
                          arrowprops={'arrowstyle': '->', 'lw': 2}, va='c
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[101]: (-4.0, 7.0, -1.0, 4.0)

- val of the grad

We can Reverse the "-"

x Pot at the min



Part 1b: Gradient Descent

Next, we will use gradients to define an important algorithm called *gradient descent*.

Calculus Review: The Gradient

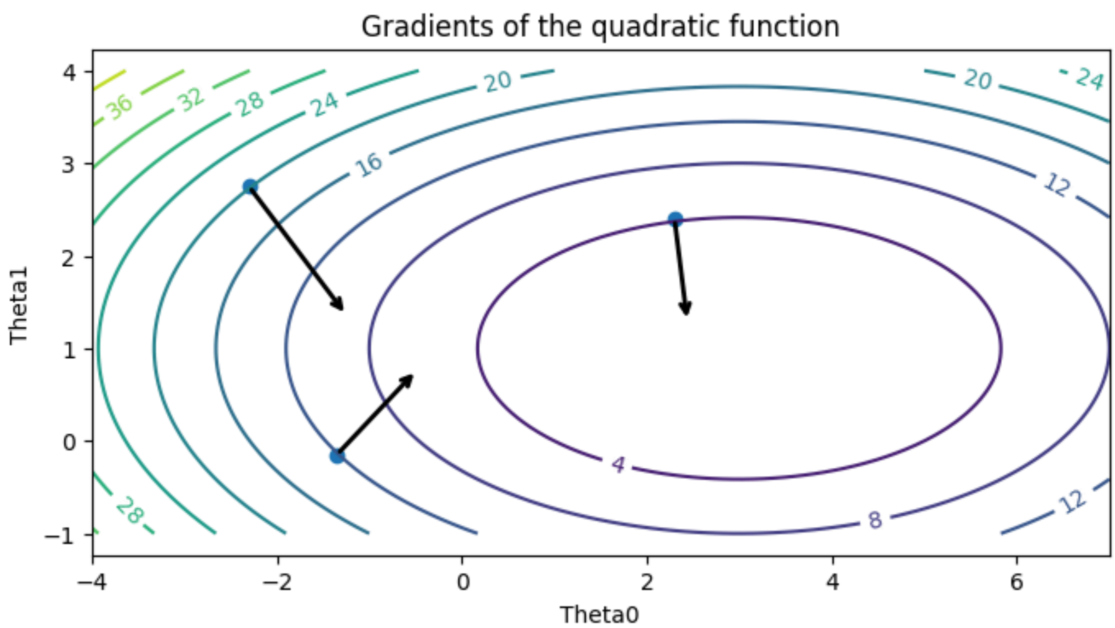
The gradient $\nabla_\theta f$ further extends the derivative to multivariate functions $f : \mathbb{R}^d \to \mathbb{R}$, and is defined at a point θ_0 as

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

The i-th entry of the vector $\nabla_\theta f(\theta_0)$ is the partial derivative $\frac{\partial f(\theta_0)}{\partial \theta_i}$ of f with respect to

In [10]:
```
theta0_pts, theta1_pts = np.array([2.3, -1.35, -2.3]), np.array([2.4
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-lin
                 arrowprops={'arrowstyle': '->', 'lw': 2}, va='c
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)
```



Gradient Descent: Intuition

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.

Slam the

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:

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

In 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)
```

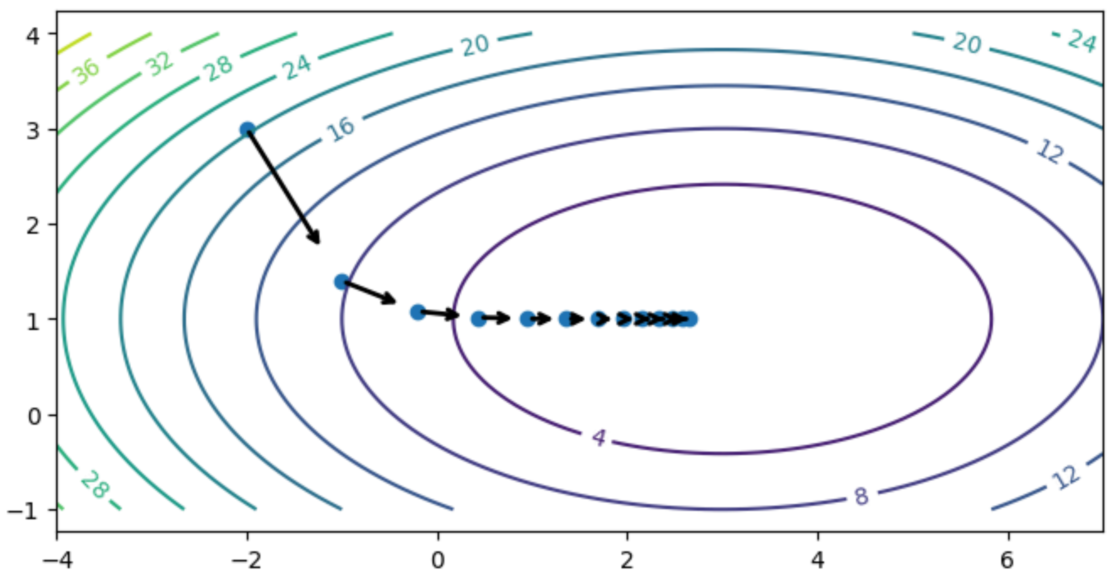
It's easy to implement this function in `numpy`.

In [108]:
```
convergence_threshold = 0.1
step_size = 0.2
theta, theta_prev = np.array([[-2], [3]]), np.array([[0], [0]])
opt_pts = [theta.flatten()]
opt_grads = []

while np.linalg.norm(theta - theta_prev) > convergence_threshold:
    # we repeat this while the value of the function is decreasing
    theta_prev = theta
    gradient = quadratic_derivative2d(*theta).reshape([2,1])
    theta = theta_prev - step_size * gradient
    opt_pts += [theta.flatten()]
    opt_grads += [gradient.flatten()]
```

We can now visualize gradient descent.

In [109]:
```
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]-
                 arrowprops={'arrowstyle': '->', 'lw': 2}, va='cente

plt.axis('equal')
```

Out[109]: (-4.0, 7.0, -1.0, 4.0)



Part 2: Gradient Descent in Linear Models

Let's now use gradient descent to derive a supervised learning algorithm for linear models.

Review: Gradient Descent

If we want to optimize $J(\theta)$, we start with an initial guess θ_0 for the parameters and repeat the following update:

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

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)
```

Review: Linear Model Family

θ are the Parameter of the 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

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

Let's define our model in Python.

In [13]:
```
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)
```

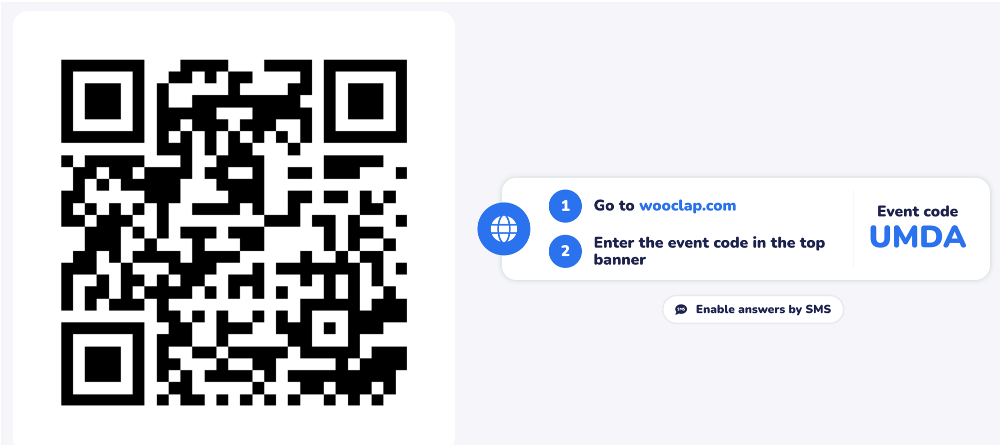
An Objective: Mean Squared Error

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.

POLL:



Here we use as an objective function the mean squared error for each training point i which is defined as $(y^{(i)} - \theta^\top x^{(i)})^2$. Would it be also okay to use the following functions?

i) $y^{(i)} - \theta^\top x^{(i)}$ All the + could eliminate the -

ii) $|y^{(i)} - \theta^\top x^{(i)}|$

Squared vs

A. yeah both

B. none of them

C. only i)

D. only ii)

E. unicorns are black

Let's implement the mean squared error.

In [110]:
```python
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)
```

Mean Squared Error: Partial Derivatives

Let's work out the derivatives for $\frac{1}{2}\left(f_\theta(x^{(i)}) - y^{(i)}\right)^2$, the MSE of a linear model f_θ for one training example $(x^{(i)}, y^{(i)})$, which we denote $J^{(i)}(\theta)$.

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

At any Point, from Jar going to rezero: = error - scaled at the value of the input at that Point

"It means don't need to rerun"

my Input for Parameter J "Scalar"

Mean Squared Error: The Gradient

We can use this derivation to obtain an expression for the gradient of the MSE for a linear model

We have 1 θ for each Feat

$$\nabla_\theta J^{(i)}(\theta) = \begin{bmatrix} \frac{\partial J^{(i)}(\theta)}{\partial \theta_0} \\ \frac{\partial J^{(i)}(\theta)}{\partial \theta_1} \\ \vdots \\ \frac{\partial J^{(i)}(\theta)}{\partial \theta_d} \end{bmatrix} = \begin{bmatrix} \left(f_\theta(x^{(i)}) - y^{(i)}\right) \cdot x_0^{(i)} \\ \left(f_\theta(x^{(i)}) - y^{(i)}\right) \cdot x_1^{(i)} \\ \vdots \\ \left(f_\theta(x^{(i)}) - y^{(i)}\right) \cdot x_d^{(i)} \end{bmatrix} = \left(f_\theta(x^{(i)}) - y^{(i)}\right) \cdot x^{(i)}$$

Computed PER DATA Pt

Note that the MSE over the entire dataset is $J(\theta) = \frac{1}{n}\sum_{i=1}^{n} J^{(i)}(\theta)$. Therefore:

$$\nabla_\theta J(\theta) = \begin{bmatrix} \frac{\partial J(\theta)}{\partial \theta_0} \\ \frac{\partial J(\theta)}{\partial \theta_1} \\ \vdots \\ \frac{\partial J(\theta)}{\partial \theta_d} \end{bmatrix} = \frac{1}{n}\sum_{i=1}^{n} \begin{bmatrix} \frac{\partial J^{(i)}(\theta)}{\partial \theta_0} \\ \frac{\partial J^{(i)}(\theta)}{\partial \theta_1} \\ \vdots \\ \frac{\partial J^{(i)}(\theta)}{\partial \theta_d} \end{bmatrix} = \frac{1}{n}\boxed{\sum_{i=1}^{n}} \left(f_\theta(x^{(i)}) - y^{(i)}\right) \cdot x^{(i)}$$

Let's implement the gradient.

In [15]:
```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)
```

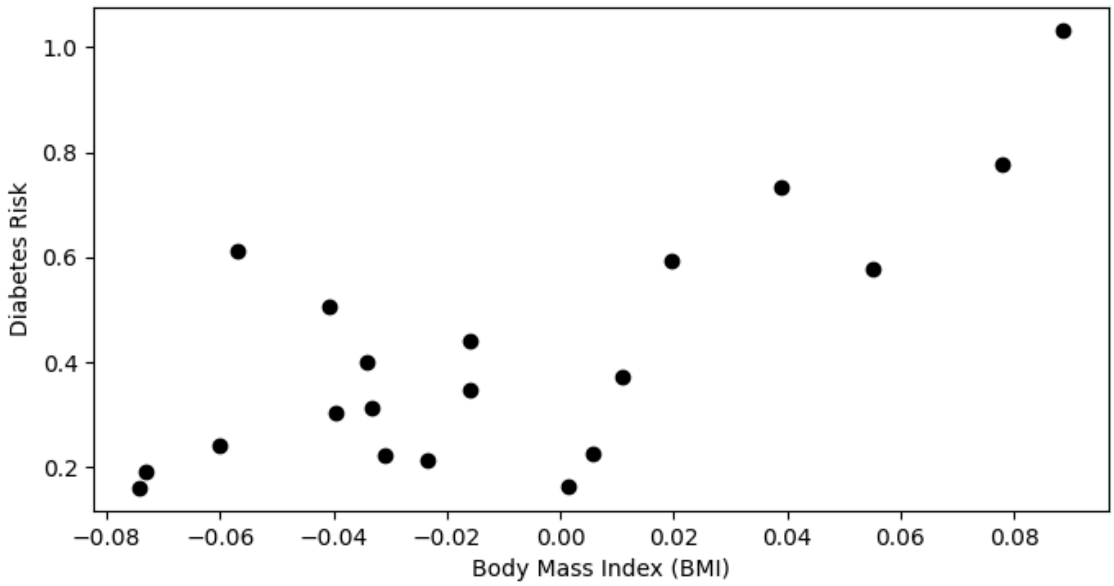
The UCI Diabetes Dataset

In this section, we are going to use the UCI Diabetes Dataset.

- 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.

In [115]:
```python
%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 ones (remember this is the X_0)
# alternatively, it's the intercept
X['one'] = 1

# Collect 20 data points and only use bmi dimension
X_train = X.iloc[-20:].loc[:, ['bmi', 'one']]
y_train = y.iloc[-20:] / 300

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

Out[115]:
```
Text(0, 0.5, 'Diabetes Risk')
```



Gradient Descent for Linear Regression

Putting this together with the gradient descent algorithm, we obtain a learning method for training linear models.

```
theta, theta_prev = random_initialization()
while abs(J(theta) - J(theta_prev)) > conv_threshold:
    theta_prev = theta
    theta = theta_prev - step_size * (f(x, theta)-y) * x
```

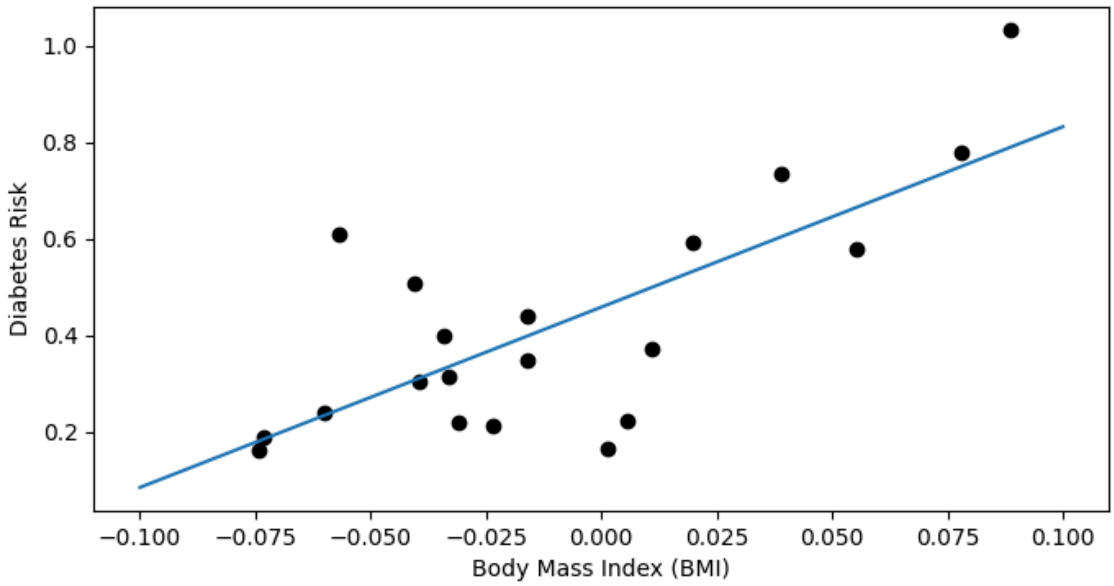
This update rule is also known as the Least Mean Squares (LMS).

In [117]:
```python
threshold = 1e-6
step_size = 4e-1
theta, theta_prev = np.array([2,1]), np.ones(2,)
opt_pts = [theta]
opt_grads = []
iter = 0

while np.linalg.norm(theta - theta_prev) > threshold:
    if iter % 100 == 0:
        print('Iteration %d. MSE: %.6f' % (iter, mean_squared_error(
    theta_prev = theta
    gradient = mse_gradient(theta, X_train, y_train)
    theta = theta_prev - step_size * gradient
    opt_pts += [theta]
    opt_grads += [gradient]
    iter += 1
```

```
Iteration 0. MSE: 0.171729
Iteration 100. MSE: 0.014765
Iteration 200. MSE: 0.014349
Iteration 300. MSE: 0.013997
Iteration 400. MSE: 0.013701
Iteration 500. MSE: 0.013450
Iteration 600. MSE: 0.013238
Iteration 700. MSE: 0.013060
Iteration 800. MSE: 0.012909
Iteration 900. MSE: 0.012781
Iteration 1000. MSE: 0.012674
Iteration 1100. MSE: 0.012583
Iteration 1200. MSE: 0.012506
Iteration 1300. MSE: 0.012441
Iteration 1400. MSE: 0.012386
Iteration 1500. MSE: 0.012340
Iteration 1600. MSE: 0.012301
Iteration 1700. MSE: 0.012268
Iteration 1800. MSE: 0.012240
```

In [126]:
```python
x_line = np.stack([np.linspace(-0.1, 0.1, 10), np.ones(10,)])
y_line = opt_pts[-1].dot(x_line)

plt.scatter(X_train.loc[:,['bmi']], y_train,  color='black')
plt.plot(x_line[0], y_line)
plt.xlabel('Body Mass Index (BMI)')
plt.ylabel('Diabetes Risk')
```

Out[126]:
```
Text(0, 0.5, 'Diabetes Risk')
```



In [125]:
```python
optimal_theta=opt_pts[-1]
print(optimal_theta)
```

```
bmi     3.736702
one     0.457953
dtype: float64
```

What do these coefficients show us?

$\theta_0 = 0.$

$$y = \theta_0 + \theta_1 \times x$$

where x is the bmi input and y is the diabetes risk.

- θ_0 $(0.457985$ in this case) is the diabetes risk for a patient with BMI 0. In the context of this problem it does not make sense. It controls the line vertically.
- θ_1 $(3.736702$ in this case) means that for every 1 unit increase in BMI, the diabetes risk increases by approx. 3.73 units. Pay attention, all units are the units that each variable is measured in when input to the model. It controls how steep is the line (angle).

Part 3: Ordinary Least Squares

We can find exactly for linear

In practice, there is a more effective way than gradient descent to find linear model parameters.

This method will produce one of the most basic algorithms: Ordinary Least Squares.

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

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

In other words, 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.

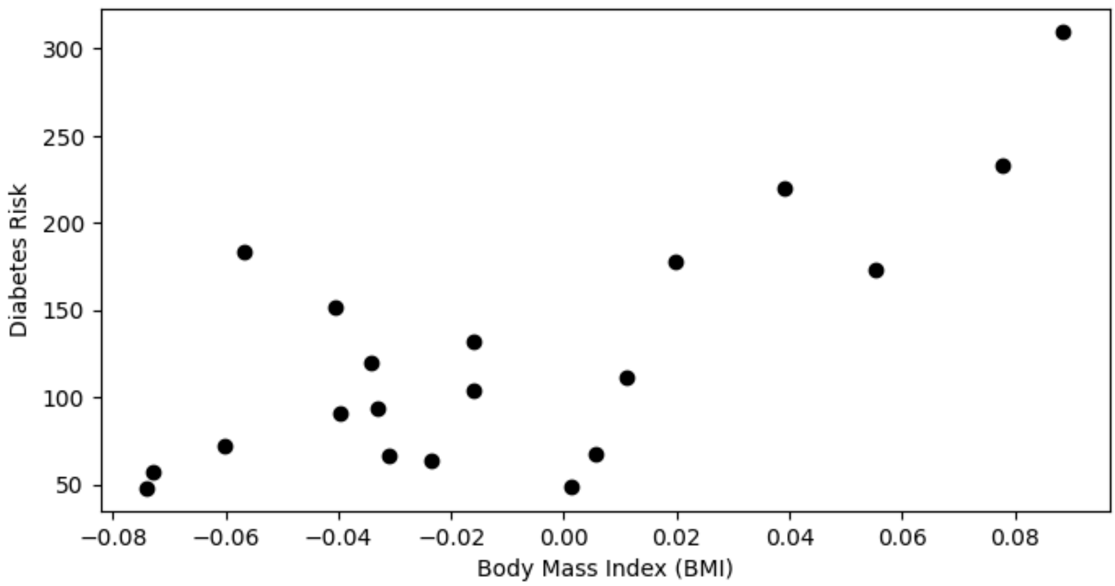
The UCI Diabetes Dataset

In this section, we are going to again use the UCI Diabetes Dataset.

- For each patient we have a access to a measurement of their body mass index (BMI) and a quantitative diabetes risk score (from 0-300).
- We are interested in understanding how BMI affects an individual's diabetes risk.

In [143]:
```python
%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[143]: Text(0, 0.5, 'Diabetes Risk')



Notation: Design 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:

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

We can view the design matrix for the diabetes dataset.

```
In [138]: X_train.head()
```

Out[138]:

	age	sex	bmi	bp	s1	s2	s3	s4
422	-0.078165	0.050680	0.077863	0.052858	0.078236	0.064447	0.026550	-0.002592
423	0.009016	0.050680	-0.039618	0.028758	0.038334	0.073529	-0.072854	0.108111
424	0.001751	0.050680	0.011039	-0.019442	-0.016704	-0.003819	-0.047082	0.034309
425	-0.078165	-0.044642	-0.040696	-0.081414	-0.100638	-0.112795	0.022869	-0.076395
426	0.030811	0.050680	-0.034229	0.043677	0.057597	0.068831	-0.032356	0.057557

Notation: Target Vector

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

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

Squared Error in Matrix Form

Recall that we may fit a linear model by choosing θ that minimizes the squared error:

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

We can write this sum in matrix-vector form as:

$$J(\theta) = \frac{1}{2}(y - X\theta)^\top (y - X\theta) = \frac{1}{2}\|y - X\theta\|^2,$$

where X is the design matrix and $\|\cdot\|$ denotes the Euclidean norm.

The Gradient of the Squared Error

We can compute the gradient of the mean squared error as follows.

$$\begin{aligned} \nabla_\theta J(\theta) &= \nabla_\theta \frac{1}{2}(X\theta - y)^\top (X\theta - y) \\ &= \frac{1}{2}\nabla_\theta \left((X\theta)^\top (X\theta) - (X\theta)^\top y - y^\top (X\theta) + y^\top y\right) \\ &= \frac{1}{2}\nabla_\theta \left(\theta^\top (X^\top X)\theta - 2(X\theta)^\top y\right) \\ &= \frac{1}{2}\left(2(X^\top X)\theta - 2X^\top y\right) \\ &= \boxed{(X^\top X)\theta - X^\top y} \end{aligned}$$

We used the facts that $a^\top b = b^\top a$ (line 3), that $\nabla_x b^\top x = b$ (line 4), and that $\nabla_x x^\top A x = 2Ax$ for a symmetric matrix A (line 4).

Normal Equations

Setting the above derivative to zero, we obtain the *normal equations*:

$$(X^\top X)\theta = X^\top y.$$

Hence, the value θ^* that minimizes this objective is given by:

$$\theta^* = (X^\top X)^{-1} X^\top y.$$

Note that we assumed that the matrix $(X^\top X)$ is invertible; there are simple ways to deal with non-invertible matrices.

Let's apply the normal equations.

In [139]:
```
import numpy as np

theta_best = np.linalg.inv(X_train.T.dot(X_train)).dot(X_train.T).dc
theta_best_df = pd.DataFrame(data=theta_best[np.newaxis, :], columns
theta_best_df
```

Out[139]:

	age	sex	bmi	bp	s1	s2	s3
0	-3.888868	204.648785	-64.289163	-262.796691	14003.726808	-11798.307781	-5892.15807

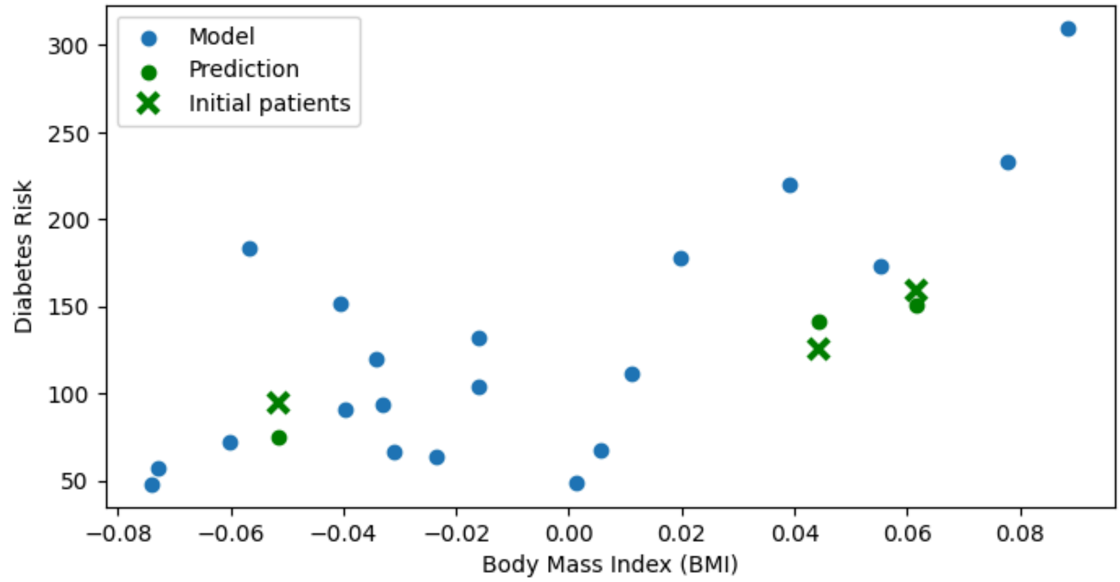
We can now use our estimate of theta to compute predictions for 3 new data points.

In [146]:
```
# Collect 3 data points for testing
X_test = X.iloc[:3]
y_test = y.iloc[:3]

# generate predictions on the new patients
y_test_pred = X_test.dot(theta_best)
```

Let's visualize these predictions.

In [147]:
```python
# visualize the results
plt.xlabel('Body Mass Index (BMI)')
plt.ylabel('Diabetes Risk')
plt.scatter(X_train.loc[:, ['bmi']], y_train)
plt.scatter(X_test.loc[:, ['bmi']], y_test, color='green', marker='o
plt.plot(X_test.loc[:, ['bmi']], y_test_pred, 'x', color='green', me
plt.legend(['Model', 'Prediction', 'Initial patients', 'New patients
```

Out[147]: <matplotlib.legend.Legend at 0x7fa6c59ca100>



Algorithm: Ordinary Least Squares

- **Type**: Supervised learning (regression)
- **Model family**: Linear models
- **Objective function**: Mean squared error
- **Optimizer**: Normal equations

It is preferred to gradient descent since it does not require any parameter tuning.

Part 4: Non-Linear Least Squares

We can extend it

So far, we have learned about a very simple linear model. Linear models can capture only simple linear relationships in the data. Can we also use it to model more complex relationships?

Review: Polynomial Functions

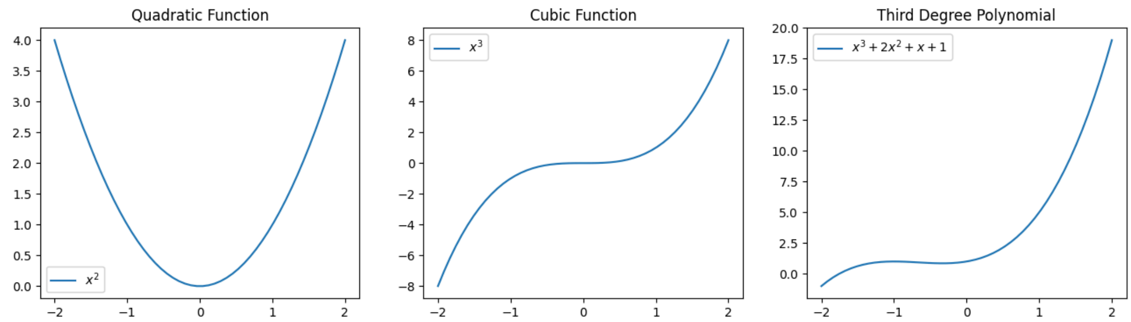
Recall that a polynomial of degree p is a function of the form

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

Below are some examples of polynomial functions.

In [148]:
```python
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[148]:
```
<matplotlib.legend.Legend at 0x7fa6c5d5f8b0>
```



Modeling Non-Linear Relationships With Polynomial Regression

Specifically, given a one-dimensional continuous variable x, we can define the *polynomial feature* function $\phi : \mathbb{R} \to \mathbb{R}^{p+1}$ as

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

The class of models of the form

$$f_\theta(x) := \sum_{j=0}^{p} \theta_j x^j = \theta^\top \boxed{\phi}(x)$$

with parameters θ and polynomial features ϕ is the set of p-degree polynomials.

- This model is non-linear in the input variable x, meaning that we can model complex data relationships.

- It is a linear model as a function of the parameters θ, meaning that we can use the ordinary least squares algorithm to learn these features.

Still Apple

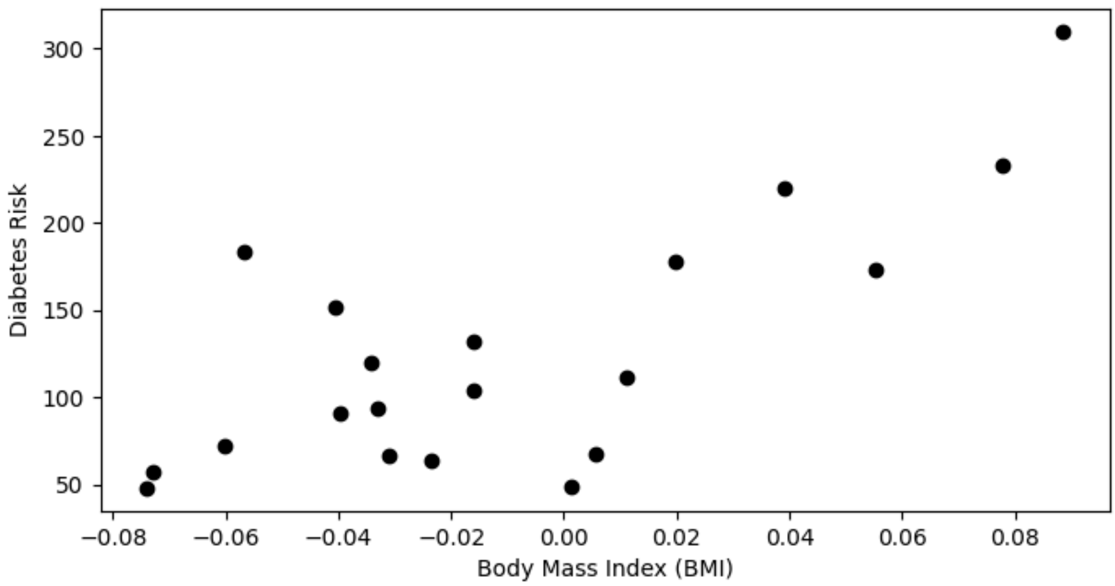
The UCI Diabetes Dataset

In this section, we are going to again use the UCI Diabetes Dataset.

- For each patient we have a access to a measurement of their body mass index (BMI) and a quantitative diabetes risk score (from 0-300).
- We are interested in understanding how BMI affects an individual's diabetes risk.

In [149]:
```
%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 ones
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[149]:
```
Text(0, 0.5, 'Diabetes Risk')
```



Diabetes Dataset: A Non-Linear Featurization

Let's now obtain linear features for this dataset.

In [150]:
```
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[150]:

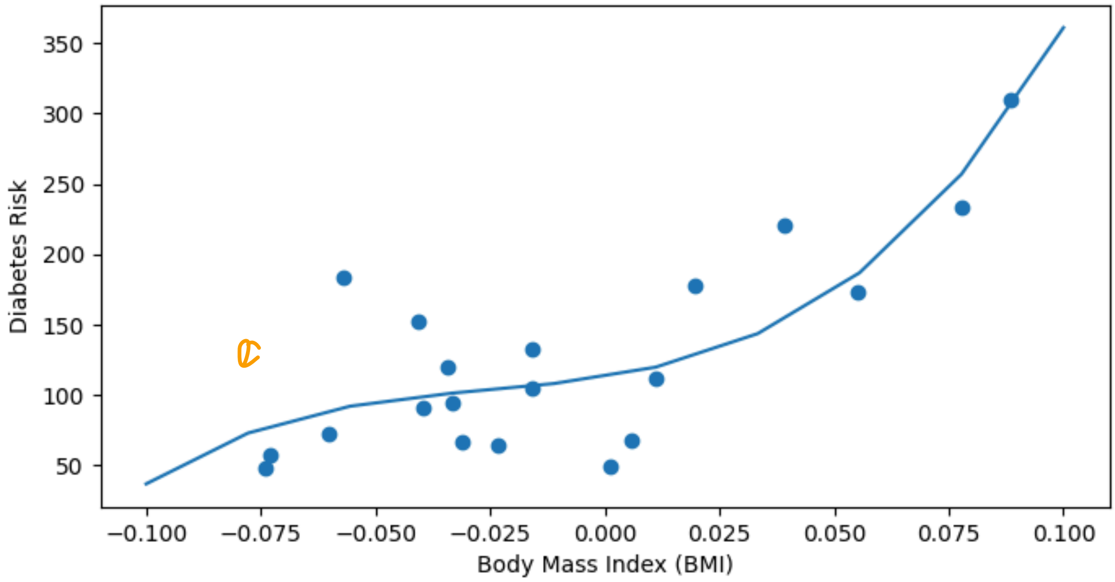
	bmi	bmi2	bmi3	one
422	0.077863	0.006063	0.000472	1
423	-0.039618	0.001570	-0.000062	1
424	0.011039	0.000122	0.000001	1
425	-0.040696	0.001656	-0.000067	1
426	-0.034229	0.001172	-0.000040	1

Diabetes Dataset: A Polynomial Model

By training a linear model on this featurization of the diabetes set, we can obtain a polynomial model of diabetes risk as a function of BMI.

In [151]:
```
# Fit a linear regression
theta = np.linalg.inv(X_bmi_p3.T.dot(X_bmi_p3)).dot(X_bmi_p3.T).dot(

# 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,)], a
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[151]:
```
[<matplotlib.lines.Line2D at 0x7fa6c3bb37f0>]
```



Multivariate Polynomial Regression

We can construct non-linear functions of multiple variables by using multivariate polynomials.

For example, a polynomial of degree 2 over two variables x_1, x_2 is a function of the form

$$a_{20} x_1^2 + a_{10} x_1 + a_{02} x_2^2 + a_{01} x_2 + a_{11} x_1 x_2 + a_{00}.$$

In general, a polynomial of degree p over two variables x_1, x_2 is a function of the form
$$f(x_1, x_2) = \sum_{i,j \geq 0 : i+j \leq p} a_{ij} x_1^i x_2^j.$$

In our two-dimensional example, this corresponds to a feature function $\phi : \mathbb{R}^2 \to \mathbb{R}^6$ of the form

$$\begin{bmatrix} 1 \\ x_1 \\ x_1^2 \end{bmatrix}$$

Towards General Non-Linear Features

Any non-linear feature map $\phi(x) : \mathbb{R}^d \to \mathbb{R}^p$ can be used in this way to obtain general models of the form

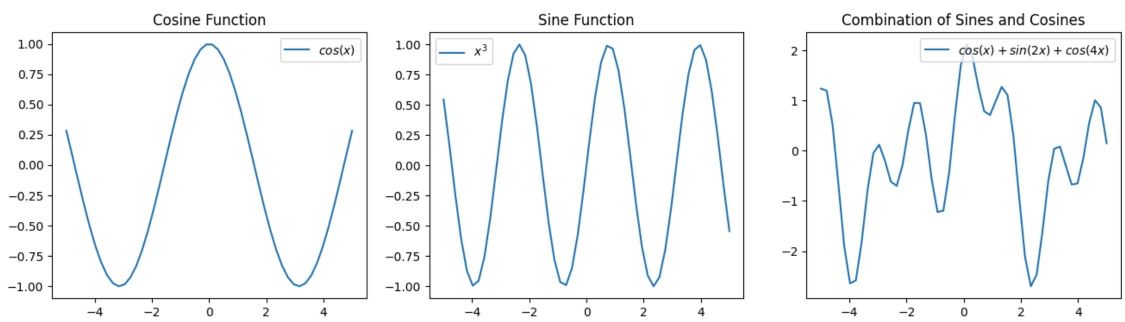
$$f_\theta(x) := \theta^\top \phi(x)$$

that are highly non-linear in x but linear in θ.

For example, here is a way of modeling complex periodic functions via a sum of sines and cosines.

In [29]:
```
import warnings
warnings.filterwarnings("ignore")

plt.figure(figsize=(16,4))
x_vars = np.linspace(-5, 5)

plt.subplot(131)
plt.title('Cosine Function')
plt.plot(x_vars, np.cos(x_vars))
plt.legend(["$cos(x)$"])

plt.subplot(132)
plt.title('Sine Function')
plt.plot(x_vars, np.sin(2*x_vars))
plt.legend(["$x^3$"])

plt.subplot(133)
plt.title('Combination of Sines and Cosines')
plt.plot(x_vars, np.cos(x_vars) + np.sin(2*x_vars) + np.cos(4*x_vars
plt.legend(["$cos(x) + sin(2x) + cos(4x)$"])
```

Out[29]:
```
<matplotlib.legend.Legend at 0x7fa6d4a489a0>
```



Part 5: Using scikit-learn to fit Multiple Linear Regression Model

Let's consider the `penguins` dataset.

In [152]:
```python
df = sns.load_dataset("penguins")
df = df[df["species"] == "Adelie"].dropna()
df
```

Out[152]:

	species	island	bill_length_mm	bill_depth_mm	flipper_length_mm	body_mass_g	
0	Adelie	Torgersen	39.1	18.7	181.0	3750.0	
1	Adelie	Torgersen	39.5	17.4	186.0	3800.0	Fe
2	Adelie	Torgersen	40.3	18.0	195.0	3250.0	Fe
4	Adelie	Torgersen	36.7	19.3	193.0	3450.0	Fe
5	Adelie	Torgersen	39.3	20.6	190.0	3650.0	
...	...	...	...	...	...	...	
147	Adelie	Dream	36.6	18.4	184.0	3475.0	Fe
148	Adelie	Dream	36.0	17.8	195.0	3450.0	Fe
149	Adelie	Dream	37.8	18.1	193.0	3750.0	
150	Adelie	Dream	36.0	17.1	187.0	3700.0	Fe
151	Adelie	Dream	41.5	18.5	201.0	4000.0	

146 rows × 7 columns

Suppose we could measure flippers and weight easily, but not bill dimensions. How can we predict **bill depth** from flipper length and/or body mass?

For demo purposes, we'll drop all columns except the variables whose relationships we're interested in modeling.

In [153]:
```python
df = sns.load_dataset("penguins")
df = df[df["species"] == "Adelie"].dropna()
df = df[["bill_depth_mm", "flipper_length_mm", "body_mass_g"]]
df
```

Out[153]:

y

	bill_depth_mm	flipper_length_mm	body_mass_g
0	18.7	181.0	3750.0
1	17.4	186.0	3800.0
2	18.0	195.0	3250.0
4	19.3	193.0	3450.0
5	20.6	190.0	3650.0
...	...	...	...
147	18.4	184.0	3475.0
148	17.8	195.0	3450.0
149	18.1	193.0	3750.0
150	17.1	187.0	3700.0
151	18.5	201.0	4000.0

146 rows × 3 columns

Suppose we want to create a linear regression model that predicts a penguin's **bill depth** y using both their **flipper length** x_1 and **body mass** x_2, plus an intercept term.

$$\hat{y} = \theta_0 + \theta_1 x_1 + \theta_2 x_2$$

Using SKLearn to fit our Multiple Linear Regression Model

An alternate approach to optimize our model is to use the `sklearn.linear_model.LinearRegression` class. [(Documentation) (https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LinearRegression.html)](https://scikit-learn.org/stable/modules/generated/sklearn.linear_model.LinearRegression.html)

In [32]:
```python
from sklearn.linear_model import LinearRegression
```

1. **Create an `sklearn` object.**

   First we create a model. At this point the model has not been fit so it has no parameters.

In [33]:
```python
from sklearn.linear_model import LinearRegression
model = LinearRegression()
model
```

Out[33]: `LinearRegression()`

2. `fit` **the object to data.**

Then we "fit" the model, which means computing the parameters that minimize the loss function. The `LinearRegression` class is hard coded to use the **MSE** as its loss function. The first argument of the fit function should be a matrix (or DataFrame), and the second should be the observations we're trying to predict.

In [34]:
```python
model.fit(
    X=df[["flipper_length_mm", "body_mass_g"]],
    y=df["bill_depth_mm"])
```

Out[34]: `LinearRegression()`

3. **Analyze fit or call** `predict` **.**

Now that our model is trained, we can ask it questions. The code below asks the model to estimate the bill depth (in mm) for a penguin with a 185 mm flipper length.

In [35]:
```python
model.predict([[185, 3750.0]]) # note the double brackets
```

Out[35]: `array([18.36187501])`

We can also ask the model to generate a series of predictions:

In [36]:
```python
df["sklearn_preds"] = model.predict(df[["flipper_length_mm", "body_m
df
```

Out[36]:

	bill_depth_mm	flipper_length_mm	body_mass_g	sklearn_preds
0	18.7	181.0	3750.0	18.322561
1	17.4	186.0	3800.0	18.445578
2	18.0	195.0	3250.0	17.721412
4	19.3	193.0	3450.0	17.997254
5	20.6	190.0	3650.0	18.263268
...	...	...	...	...
147	18.4	184.0	3475.0	17.945735
148	17.8	195.0	3450.0	18.016911
149	18.1	193.0	3750.0	18.440503
150	17.1	187.0	3700.0	18.307657
151	18.5	201.0	4000.0	18.888505

146 rows × 4 columns

Voilà!

Analyze parameters.

We can ask the model for its intercept and slope with `_intercept` and `_coef` , respectively.

In [37]:
```python
model.intercept_      # why is this a scalar?
```

Out[37]:
```
11.002995277447067
```

In [38]:
```python
model.coef_           # why is this an array?
```

Out[38]:
```
array([0.00982849, 0.0014775 ])
```

How are these interpreted?

$$\hat{y} = \theta_0 + \theta_1 x_1 + \theta_2 x_2$$

θ_0 is the bill depth of a penguin with 0 mm flipper length and 0 grams mass weight. doesn't make sense

θ_1 is how many mm longer is the bill depth, if we increase the flipper length by 1 mm and keeping the mass ~~fixed~~. fixed

θ_2 is how many mm longer is the bill depth, if we increase the weight by 1 gram and keeping the flipper length fixed.

Analyze performance.

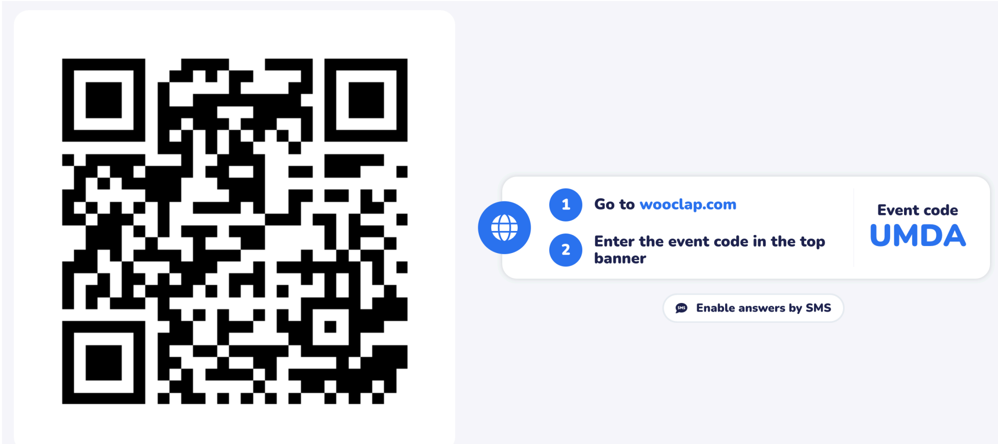
The `sklearn` package also provides a function that computes the MSE from a list of observations and predictions. This avoids us having to manually compute MSE by first computing residuals. In the second part of class, we will explore more metrics to assess model performance.

[documentation (https://scikit-learn.org/stable/modules/generated/sklearn.metrics.mean_squared_error.html)](https://scikit-learn.org/stable/modules/generated/sklearn.metrics.mean_squared_error.html)

In [39]:
```python
from sklearn.metrics import  mean_squared_error
mean_squared_error(df["bill_depth_mm"], df["sklearn_preds"])
```

Out[39]:
```
0.9764070438844
```

POLL:



Is 0.9764 a high value for the squared error?

A. Yes

How Small is Small

B. No

C. Can't say for sure

D. Unicorns are white

Part 5: Feature Engineering

Feature engineering is the process of applying feature functions to generate new features for use in modeling. We will discuss two aspects:

- One-hot encoding
- Polynomial features

To do so, we will use a dataset from seaborn, `tips`

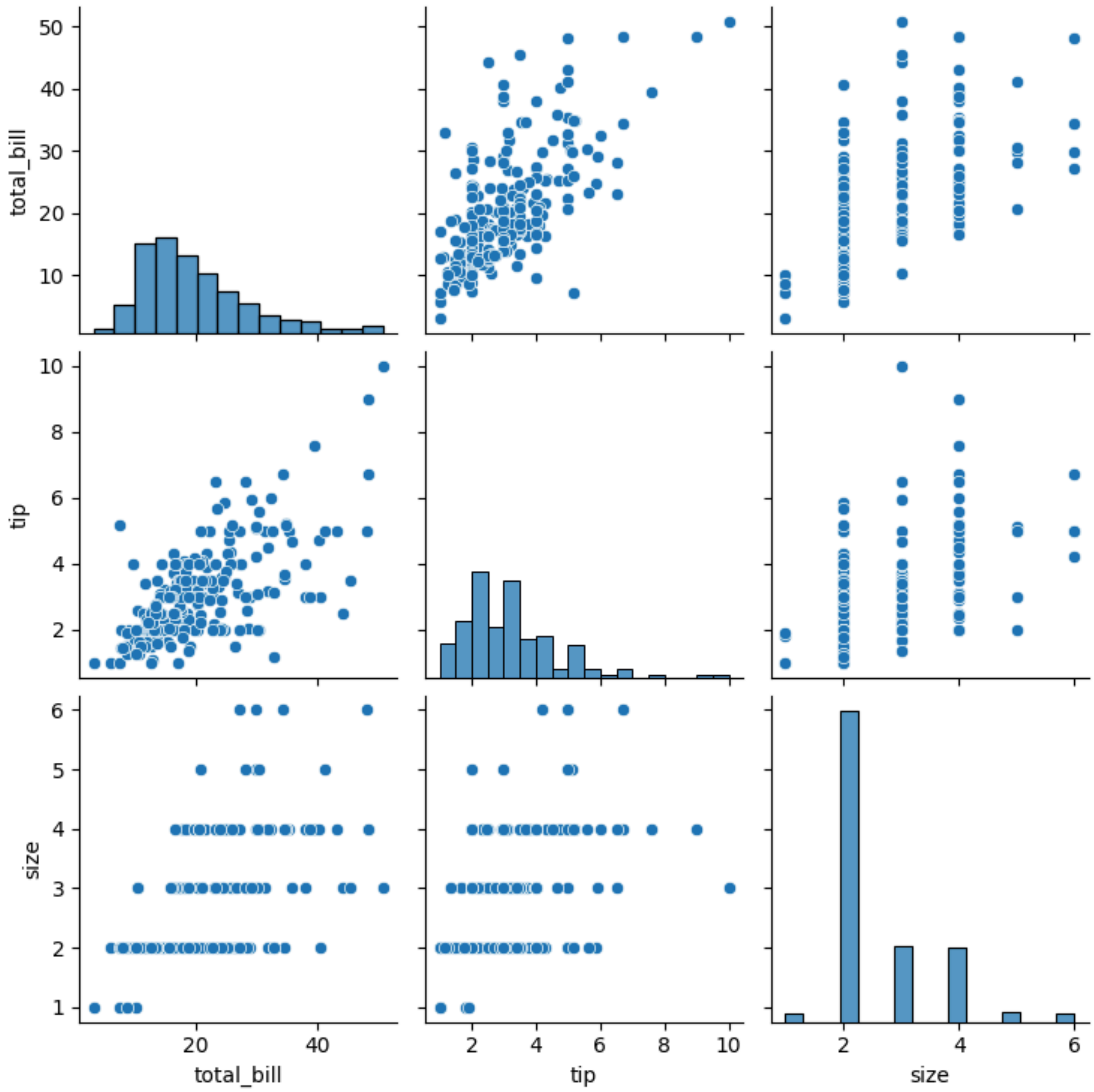
In [154]:
```
import seaborn as sns
import warnings
import plotly.express as px
import plotly.graph_objects as go
pd.options.mode.chained_assignment = None
warnings.simplefilter(action='ignore', category=UserWarning)
np.random.seed(42)

tips = sns.load_dataset("tips")
tips.head()
```

Out[154]:

	total_bill	tip	sex	smoker	day	time	size
0	16.99	1.01	Female	No	Sun	Dinner	2
1	10.34	1.66	Male	No	Sun	Dinner	3
2	21.01	3.50	Male	No	Sun	Dinner	3
3	23.68	3.31	Male	No	Sun	Dinner	2
4	24.59	3.61	Female	No	Sun	Dinner	4

In [156]:
```
sns.pairplot(tips)
```

Out[156]: <seaborn.axisgrid.PairGrid at 0x7fa6c83ab490>



One-Hot Encoding

day vs Nat Numere

We discussed One-Hot Encoding as part of EDA. Here, e.g. we can use one-hot encoding to incorporate the day of the week as an input into a regression model.

Suppose we want to use a design matrix of three features – the `total_bill`, `size`, and `day` – to predict the tip.

In [157]:
```
X_raw = tips[["total_bill", "size", "day"]]
y = tips["tip"]
```

Because `day` is non-numeric, we will apply one-hot encoding before fitting a model.

The `OneHotEncoder` class of `sklearn` ([documentation (https://scikit-learn.org/stable/modules/generated/sklearn.preprocessing.OneHotEncoder.html#sklearn.pr](https://scikit-learn.org/stable/modules/generated/sklearn.preprocessing.OneHotEncoder.html#sklearn.pr) offers a quick way to perform one-hot encoding. Also, note that we follow a very similar workflow to when we were working with the `LinearRegression` class: we initialize a `OneHotEncoder` object, fit it to our data, then use `.transform` to apply the fitted encoder.

In [158]:
```
from sklearn.preprocessing import OneHotEncoder

# Initialize a OneHotEncoder object
ohe = OneHotEncoder()

# Fit the encoder
ohe.fit(tips[["day"]])
ohe
```

Out[158]:
```
OneHotEncoder()
```

In [159]:
```
# Use the encoder to transform the raw "day" feature
encoded_day = ohe.transform(tips[["day"]]).toarray()

print("The first 5 rows of the matrix")
encoded_day[:5, :]
```

```
The first 5 rows of the matrix
```

Out[159]:
```
array([[0., 0., 1., 0.],
       [0., 0., 1., 0.],
       [0., 0., 1., 0.],
       [0., 0., 1., 0.],
       [0., 0., 1., 0.]])
```

In [161]:
```
#ohe.transform([['Fun']])
```

In [162]:
```
encoded_day_df = pd.DataFrame(encoded_day, columns=ohe.get_feature_r
encoded_day_df.head()
```

Out[162]:

	day_Fri	day_Sat	day_Sun	day_Thur
0	0.0	0.0	1.0	0.0
1	0.0	0.0	1.0	0.0
2	0.0	0.0	1.0	0.0
3	0.0	0.0	1.0	0.0
4	0.0	0.0	1.0	0.0

The `OneHotEncoder` has converted the categorical `day` feature into four numeric features! Note that the `tips` dataset only included data for Thursday through Sunday, which is why only four days of the week appear.

Let's join this one-hot encoding to the original data to form our featurized design matrix. We drop the original `day` column so our design matrix only includes numeric values.

In [163]:
```
X = X_raw.join(encoded_day_df).drop(columns="day")

X.head()
```

Out[163]:

	total_bill	size	day_Fri	day_Sat	day_Sun	day_Thur
0	16.99	2	0.0	0.0	1.0	0.0
1	10.34	3	0.0	0.0	1.0	0.0
2	21.01	3	0.0	0.0	1.0	0.0
3	23.68	2	0.0	0.0	1.0	0.0
4	24.59	4	0.0	0.0	1.0	0.0

Now, we can use `sklearn`'s `LinearRegression` class to fit a model to this design matrix.

In [164]:
```python
from sklearn.linear_model import LinearRegression
ohe_model = LinearRegression(fit_intercept=False) # Tell sklearn to
ohe_model.fit(X, y)

pd.DataFrame({"Feature":X.columns, "Model Coefficient":ohe_model.coe
```

Out[164]:

Feature	Model Coefficient
total_bill	0.092994
size	0.187132
day_Fri	0.745787
day_Sat	0.621129
day_Sun	0.732289
day_Thur	0.668294

We can use

Polynomial Features

Consider the `vehicles` dataset, which includes information about cars.

In [171]:
```python
vehicles = sns.load_dataset("mpg").dropna().rename(columns = {"horse
vehicles.head()
```

Out[171]:

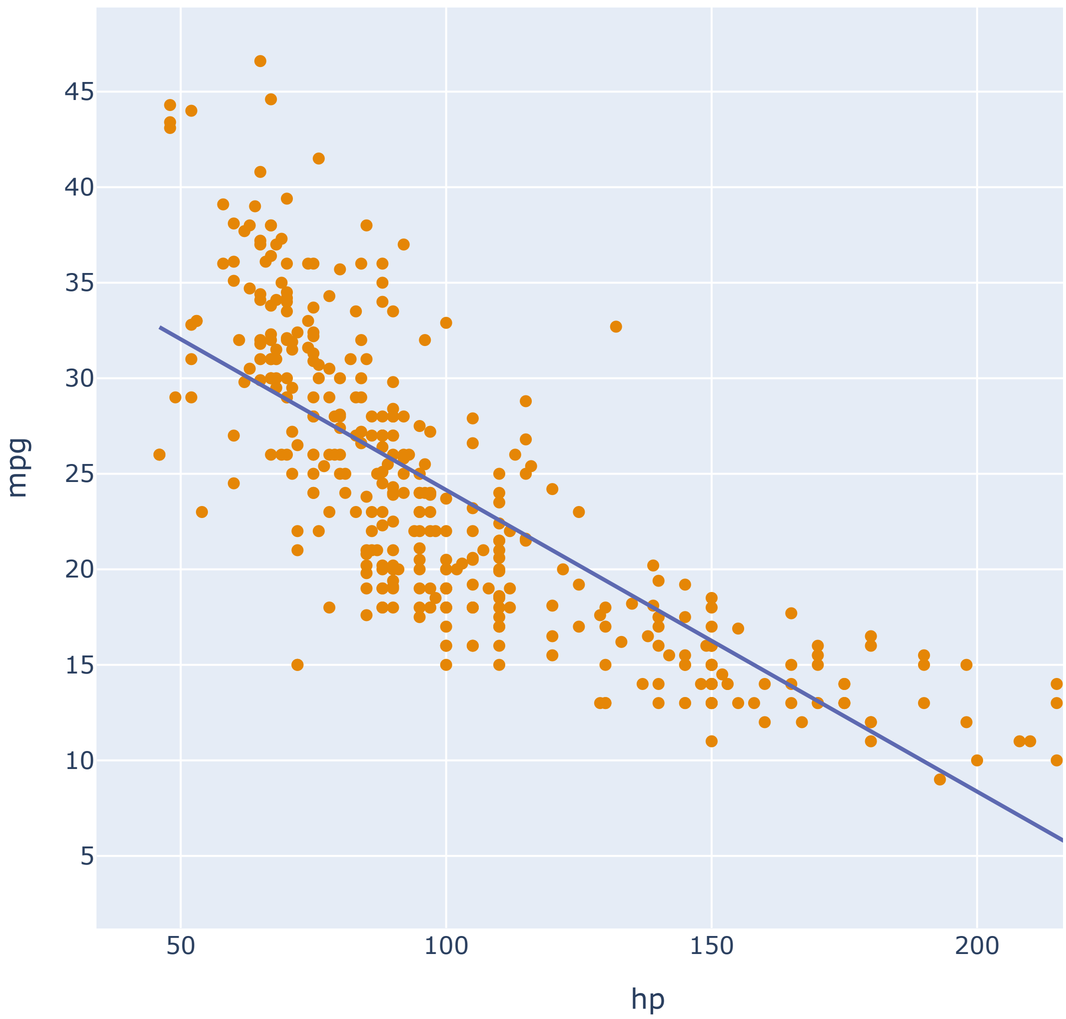
	mpg	cylinders	displacement	hp	weight	acceleration	model_year	origin	na
19	26.0	4	97.0	46.0	1835	20.5	70	europe	volkswag 1 delu sec
102	26.0	4	97.0	46.0	1950	21.0	73	europe	volkswag su bee
326	43.4	4	90.0	48.0	2335	23.7	80	europe	vw das (die
325	44.3	4	90.0	48.0	2085	21.7	80	europe	vw rabb (die
244	43.1	4	90.0	48.0	1985	21.5	78	europe	volkswag rak cust die

Suppose we want to use the `hp` (horsepower) of a car to predict its `mpg` (gas mileage in miles per gallon). If we visualize the relationship between these two variables, we see a non-linear curvature. Fitting a linear model to these variables results in a high (poor) value of RMSE.

$$\hat{y} = \theta_0 + \theta_1(\text{hp})$$

In [172]:
```
X = vehicles[["hp"]]
y = vehicles["mpg"]

hp_model = LinearRegression()
hp_model.fit(X, y)
hp_model_predictions = hp_model.predict(X)

print(f"MSE of model with (hp) feature: {np.mean((y-hp_model_predict

fig = px.scatter(vehicles, x="hp", y="mpg", width=800, height=600)
fig.add_trace(go.Scatter(x=vehicles["hp"], y=hp_model_predictions,
                         mode="lines", name="Linear Prediction"))
#sns.scatterplot(data=vehicles, x="hp", y="mpg")
#plt.plot(vehicles["hp"], hp_model_predictions, c="tab:red");
```

```
MSE of model with (hp) feature: 23.943662938603108
```

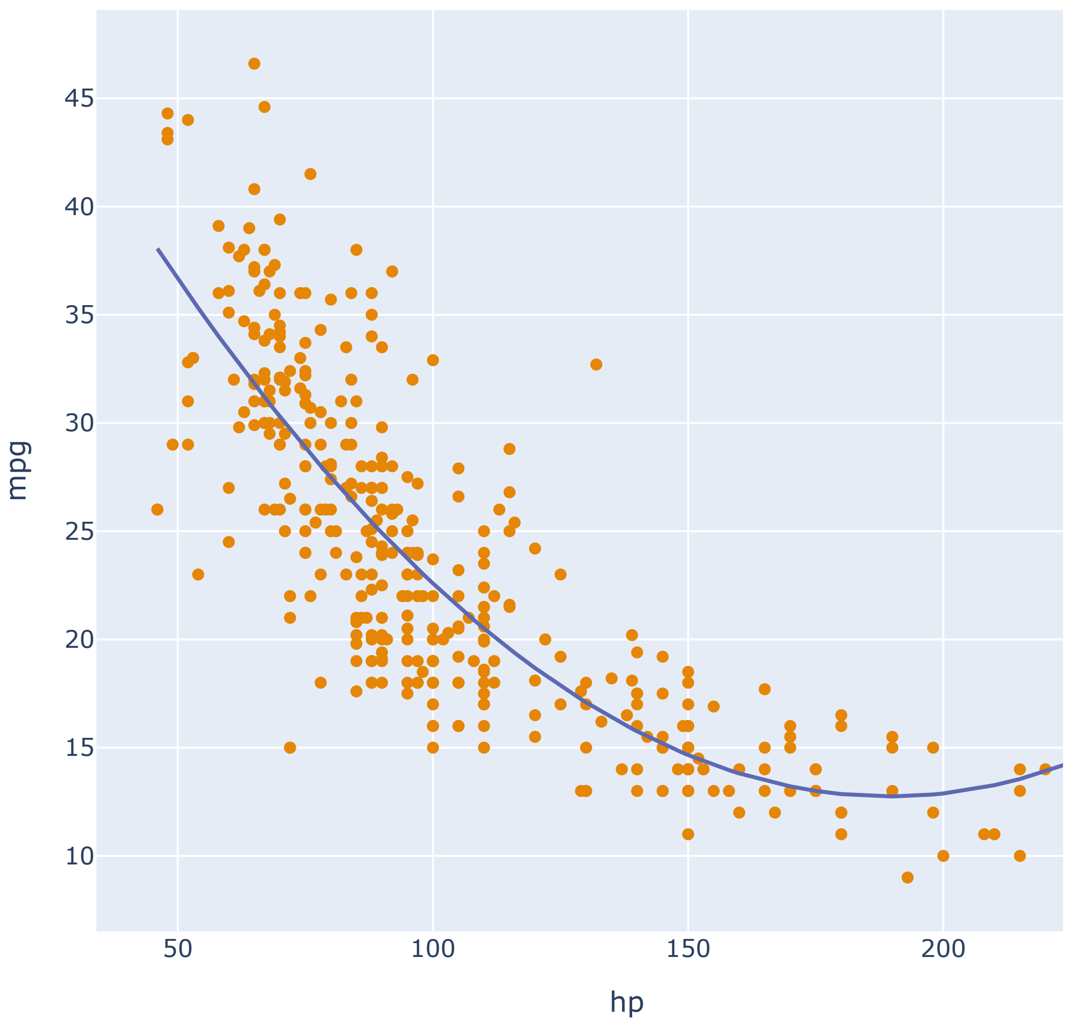


To capture the non-linear relationship between the variables, we can introduce a non-linear feature: hp squared. Our new model is:

$$\hat{y} = \theta_0 + \theta_1(\text{hp}) + \theta_2(\text{hp}^2)$$

In [173]:
```
X = vehicles[["hp"]]
X.loc[:, "hp^2"] = vehicles["hp"]**2

hp2_model = LinearRegression()
hp2_model.fit(X, y)
hp2_model_predictions = hp2_model.predict(X)


print(f"MSE of model with (hp^2) feature: {np.mean((y-hp2_model_prec

fig = px.scatter(vehicles, x="hp", y="mpg", width=800, height=600)
fig.add_trace(go.Scatter(x=vehicles["hp"], y=hp2_model_predictions,
                         mode="lines", name="Quadratic Prediction"))
#sns.scatterplot(data=vehicles, x="hp", y="mpg")
#plt.plot(vehicles["hp"], hp2_model_predictions, c="tab:red");
```

```
MSE of model with (hp^2) feature: 18.984768907617216
```



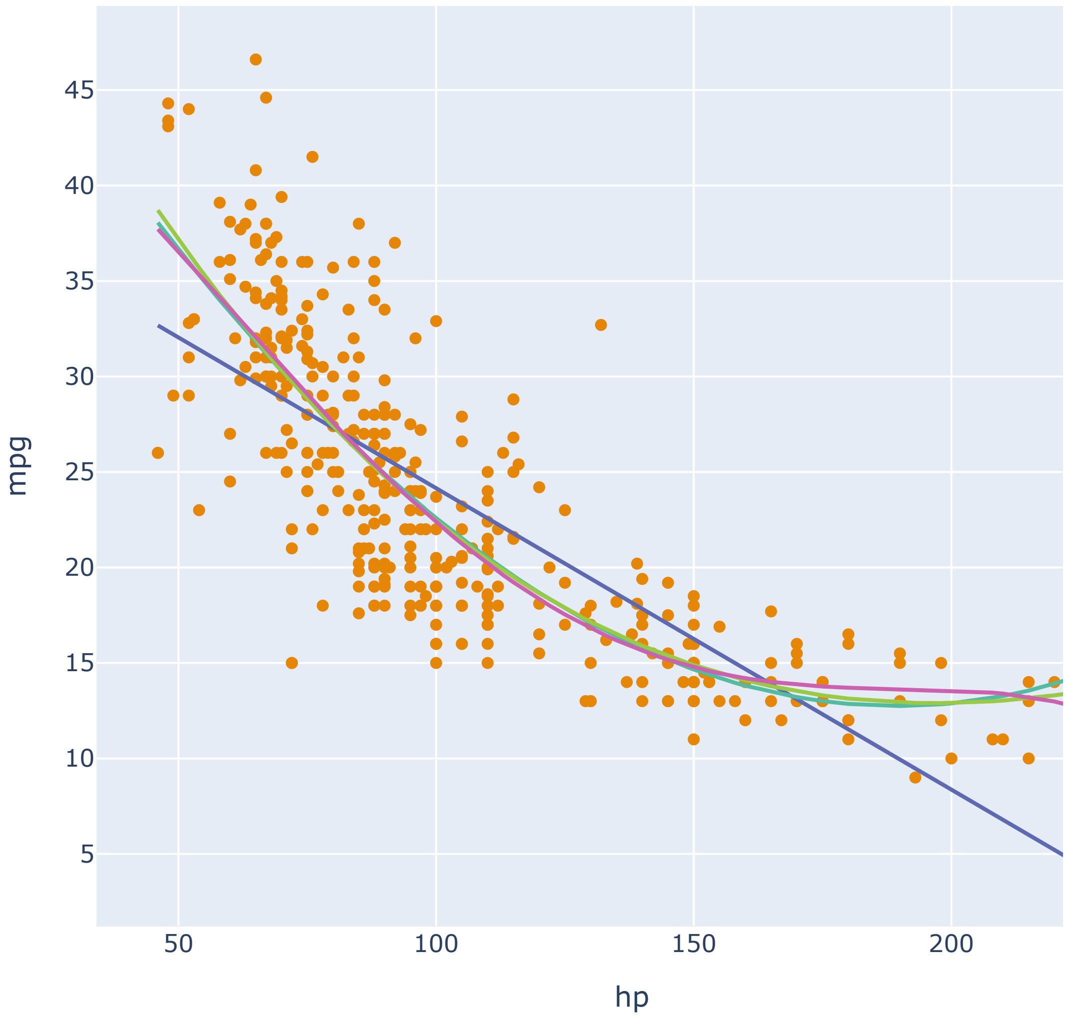
What if we take things further and add even *more* polynomial features?

The cell below fits models of increasing complexity and computes their MSEs.

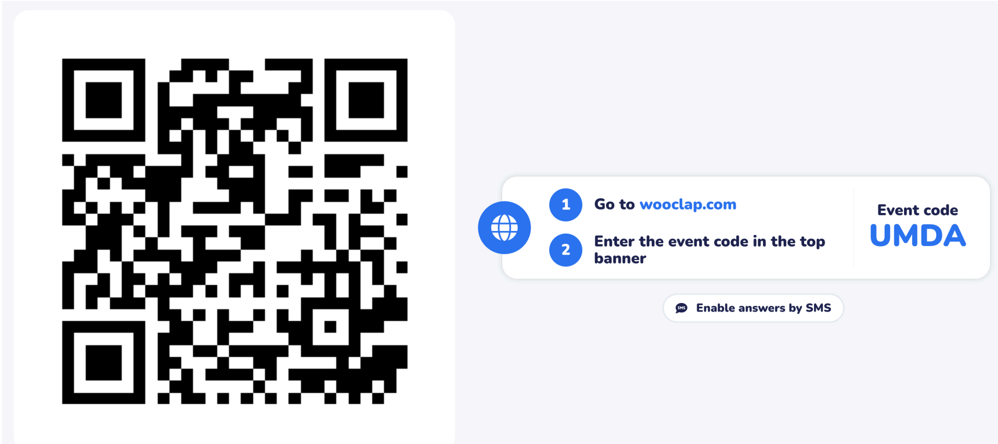
In [174]:

```
def mse(predictions, observations):
    return np.mean((observations - predictions)**2)

# Add hp^3 and hp^4 as features to the data
X["hp^3"] = vehicles["hp"]**3
X["hp^4"] = vehicles["hp"]**4

# Fit a model with order 3
hp3_model = LinearRegression()
hp3_model.fit(X[["hp", "hp^2", "hp^3"]], vehicles["mpg"])
hp3_model_predictions = hp3_model.predict(X[["hp", "hp^2", "hp^3"]])

# Fit a model with order 4
hp4_model = LinearRegression()
hp4_model.fit(X[["hp", "hp^2", "hp^3", "hp^4"]], vehicles["mpg"])
hp4_model_predictions = hp4_model.predict(X[["hp", "hp^2", "hp^3", "
```

In [175]:
```python
#Visualizing differently:
fig = px.scatter(vehicles, x="hp", y="mpg", width=800, height=600)
fig.add_trace(go.Scatter(
    x=vehicles["hp"], y=hp_model_predictions, mode="lines",
    name=f"HP MSE={np.round(mse(vehicles['mpg'], hp_model_predictior
fig.add_trace(go.Scatter(
    x=vehicles["hp"], y=hp2_model_predictions, mode="lines",
    name=f"HP^2 MSE={np.round(mse(vehicles['mpg'], hp2_model_predict
fig.add_trace(go.Scatter(
    x=vehicles["hp"], y=hp3_model_predictions, mode="lines",
    name=f"HP^3 MSE={np.round(mse(vehicles['mpg'], hp3_model_predict
fig.add_trace(go.Scatter(
    x=vehicles["hp"], y=hp4_model_predictions, mode="lines",
    name=f"HP^4 MSE={np.round(mse(vehicles['mpg'], hp4_model_predict
```



POLL:



Which model would you prefer?

A. degree 1

B. degree 2

C. degree 3

D. degree 4

E. Unicorns are blue

In [67]:
```
# Plot the models' predictions
#fig, ax = plt.subplots(1, 3, dpi=200, figsize=(12, 3))
#
#predictions_dict = {0:hp2_model_predictions, 1:hp3_model_predictior
#
#for i in predictions_dict:
#    ax[i].scatter(vehicles["hp"], vehicles["mpg"], edgecolor="white
#    ax[i].plot(vehicles["hp"], predictions_dict[i], "tab:green")
#    ax[i].set_title(f"Model with order {i+2}")
#    ax[i].set_xlabel("hp")
#    ax[i].set_ylabel("mpg")
#    ax[i].annotate(f"MSE: {np.round(mse(vehicles['mpg'], predictior
#
#plt.subplots_adjust(wspace=0.3);
```

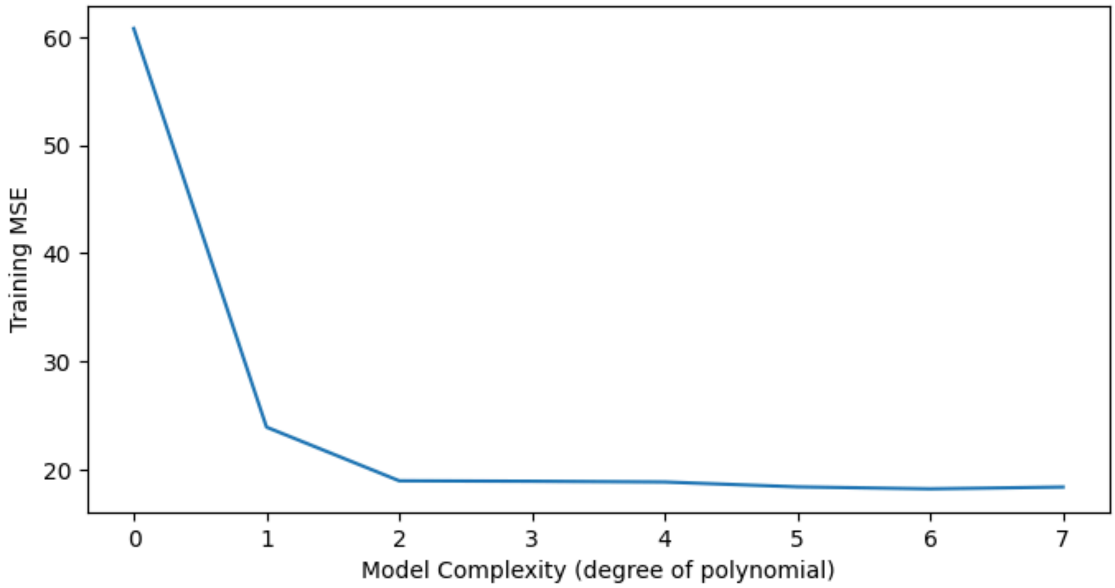
Complexity and Overfitting

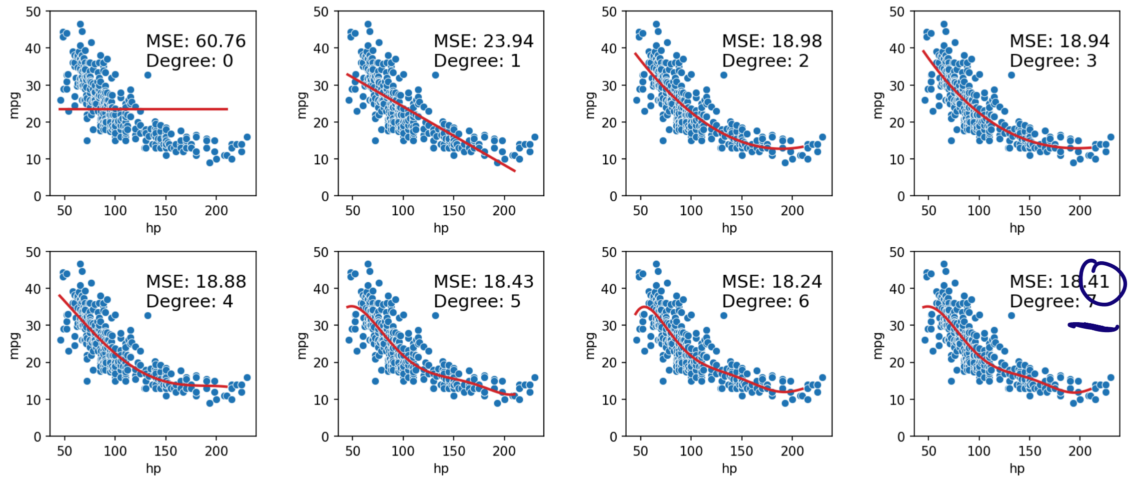
What we saw above was the phenomenon of **model complexity** – as we add additional features to the design matrix, the model becomes increasingly *complex*. Models with higher complexity have lower values of training error. Intuitively, this makes sense: with more features at its disposal, the model can match the observations in the trainining data more and more closely.

We can run an experiment to see this in action. In the cell below, we fit many models of progressively higher complexity, then plot the MSE of predictions on the training set.

The **order** of a polynomial model is the highest power of any term in the model. An order 0 model takes the form $\hat{y} = \theta_0$, while an order 4 model takes the form

In [176]:
```python
from sklearn.pipeline import Pipeline
from sklearn.preprocessing import PolynomialFeatures

def fit_model_dataset(degree, dataset):
    pipelined_model = Pipeline([
            ('polynomial_transformation', PolynomialFeatures(degree)
            ('linear_regression', LinearRegression())
        ])

    pipelined_model.fit(dataset[["hp"]], dataset["mpg"])
    return mse(dataset['mpg'], pipelined_model.predict(dataset[["hp"

errors = [fit_model_dataset(degree, vehicles) for degree in range(0,
MSEs_and_k = pd.DataFrame({"k": range(0, 8), "MSE": errors})

plt.plot(range(0, 8), errors)
plt.xlabel("Model Complexity (degree of polynomial)")
plt.ylabel("Training MSE");

def plot_degree_k_model(k, MSEs_and_k, axs):
    pipelined_model = Pipeline([
        ('poly_transform', PolynomialFeatures(degree = k)),
        ('regression', LinearRegression(fit_intercept = True))
    ])
    pipelined_model.fit(vehicles[["hp"]], vehicles["mpg"])

    row = k // 4
    col = k % 4
    ax = axs[row, col]

    sns.scatterplot(data=vehicles, x='hp', y='mpg', ax=ax)

    x_range = np.linspace(45, 210, 100).reshape(-1, 1)
    ax.plot(x_range, pipelined_model.predict(pd.DataFrame(x_range, c

    ax.set_ylim((0, 50))
    mse_str = f"MSE: {MSEs_and_k.loc[k, 'MSE']:.4}\nDegree: {k}"
    ax.text(130, 35, mse_str, dict(size=14))

fig = plt.figure(figsize=(15, 6), dpi=150)
axs = fig.subplots(nrows=2, ncols=4)

for k in range(8):
    plot_degree_k_model(k, MSEs_and_k, axs)
fig.subplots_adjust(wspace=0.4, hspace=0.3)
```





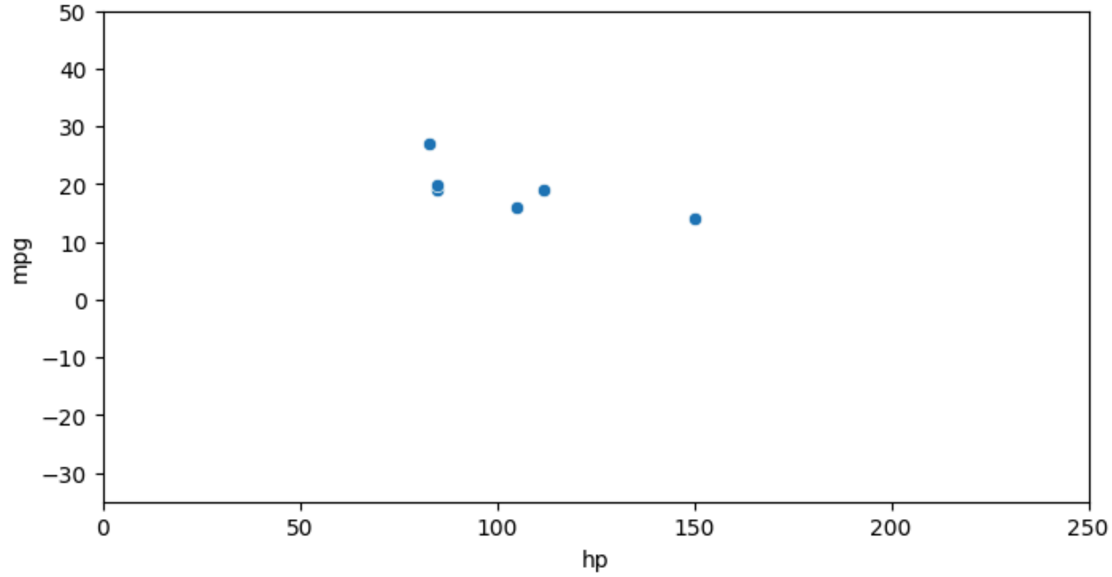
You may be tempted to always design models with high polynomial degree – after all, we know that we could theoretically achieve perfect predictions by creating a model with enough polynomial features.

It turns out that the examples we looked at above represent a somewhat artificial scenario: we trained our model on all the data we had available, then used the model to make predictions on this very same dataset. A more realistic situation is when we wish to apply our model on unseen data – that is, datapoints that it did not encounter during the model fitting process.

Suppose we obtain a random sample of 6 datapoints from our population of vehicle data. We want to train a model on these 6 points and use it to make predictions on unseen data (perhaps cars for which we don't already know the true `mpg`).

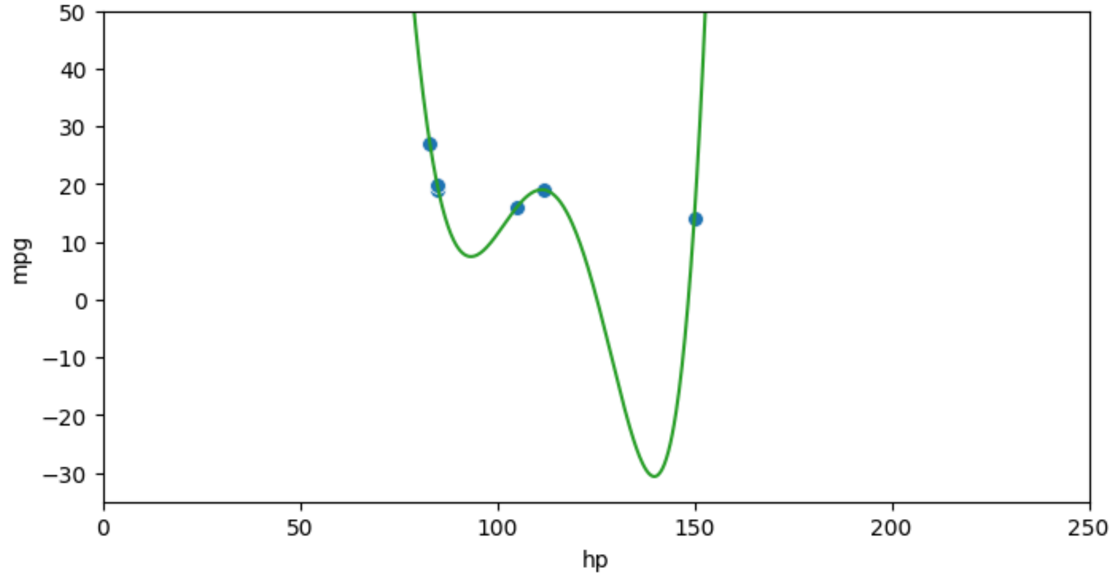
In [177]:

```
np.random.seed(100)

sample_6 = vehicles.sample(6)

sns.scatterplot(data=sample_6, x="hp", y="mpg")
plt.ylim(-35, 50)
plt.xlim(0, 250);
```



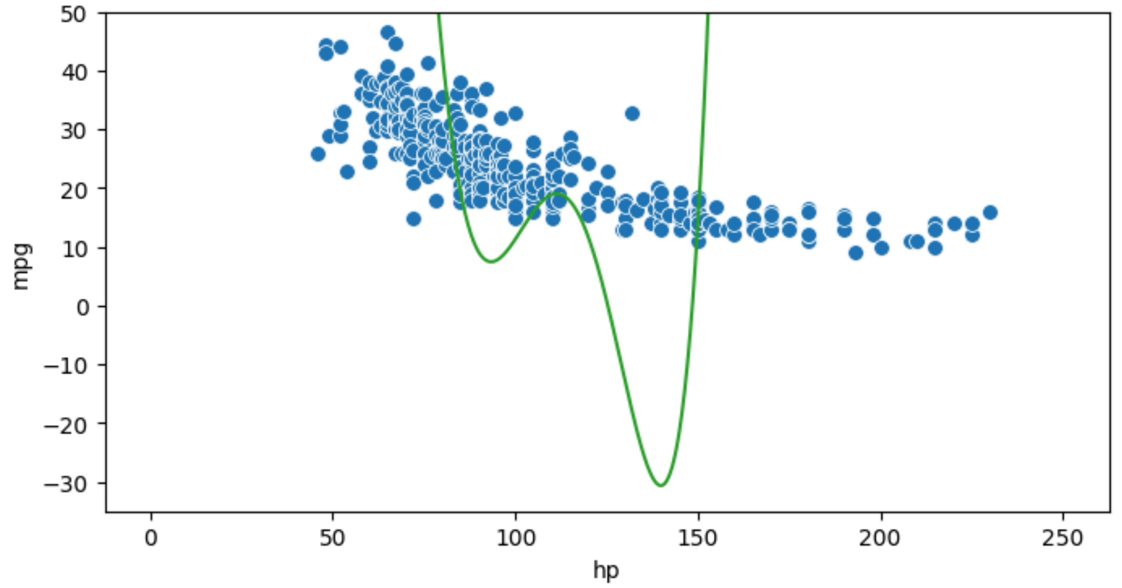
If we design a model with polynomial degree 5, we can make perfect predictions on this sample of training data.

In [56]:
```python
degree_5_model = Pipeline([
                ('polynomial_transformation', PolynomialFeatures(5)),
                ('linear_regression', LinearRegression())
            ])

degree_5_model.fit(sample_6[["hp"]], sample_6["mpg"])
xs = np.linspace(0, 250, 1000)
degree_5_model_predictions = degree_5_model.predict(xs[:, np.newaxis

plt.plot(xs, degree_5_model_predictions, c="tab:green")
sns.scatterplot(data=sample_6, x="hp", y="mpg", s=50)
plt.ylim(-35, 50)
plt.xlim(0, 250);
```



However, when we reapply this fitted model to the full population of data, it fails to capture the major trends of the dataset.

In [57]:
```python
plt.plot(xs, degree_5_model_predictions, c="tab:green")
sns.scatterplot(data=vehicles, x="hp", y="mpg", s=50)
plt.ylim(-35, 50);
```

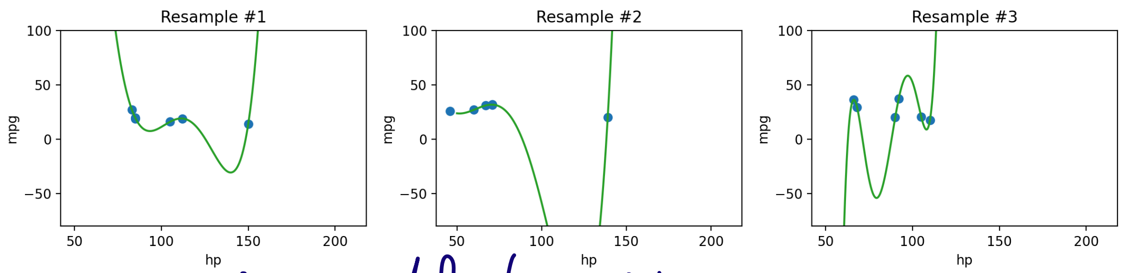


Vance Jones

The model has **overfit** to the data used to train it. It has essentially "memorized" the six datapoints used during model fitting, and does not generalize well to new data.

Complex models tend to be more sensitive to the data used to train them. The **variance** of a model refers to its tendency to vary depending on the training data used during model fitting. It turns out that our degree-5 model has very high model variance. If we randomly sample new sets of datapoints to use in training, the model varies erratically.

In [58]:
```
np.random.seed(100)

fig, ax = plt.subplots(1, 3, dpi=200, figsize=(12, 3))

for i in range(0, 3):
    sample = vehicles.sample(6)

    polynomial_model = Pipeline([
                ('polynomial_transformation', PolynomialFeatures(5))
                ('linear_regression', LinearRegression())
            ])

    polynomial_model.fit(sample[["hp"]], sample["mpg"])

    ax[i].scatter(sample[["hp"]], sample["mpg"])

    xs = np.linspace(50, 210, 1000)
    ax[i].plot(xs, polynomial_model.predict(xs[:, np.newaxis]), c="t
    ax[i].set_ylim(-80, 100)
    ax[i].set_xlabel("hp")
    ax[i].set_ylabel("mpg")
    ax[i].set_title(f"Resample #{i+1}")

fig.tight_layout();
```



This model has ↑ Var

Algorithm: Non-Linear Least Squares

- **Type**: Supervised learning (regression)
- **Model family**: Linear in the parameters; non-linear with respect to raw inputs.
- **Features**: Non-linear functions of the attributes (one-hot encoding and polynomails)
- **Objective function**: Mean squared error
- **Optimizer**: Normal equations (or Gradient Descent)