

CHAPTER 4

Training Models

So far we have treated Machine Learning models and their training algorithms mostly like black boxes. If you went through some of the exercises in the previous chapters, you may have been surprised by how much you can get done without knowing anything about what's under the hood: you optimized a regression system, you improved a digit image classifier, and you even built a spam classifier from scratch—all this without knowing how they actually work. Indeed, in many situations you don't really need to know the implementation details.

However, having a good understanding of how things work can help you quickly home in on the appropriate model, the right training algorithm to use, and a good set of hyperparameters for your task. Understanding what's under the hood will also help you debug issues and perform error analysis more efficiently. Lastly, most of the topics discussed in this chapter will be essential in understanding, building, and training neural networks (discussed in [Part II](#) of this book).

In this chapter, we will start by looking at the Linear Regression model, one of the simplest models there is. We will discuss two very different ways to train it:

- Using a direct “closed-form” equation that directly computes the model parameters that best fit the model to the training set (i.e., the model parameters that minimize the cost function over the training set).
- Using an iterative optimization approach, called Gradient Descent (GD), that gradually tweaks the model parameters to minimize the cost function over the training set, eventually converging to the same set of parameters as the first method. We will look at a few variants of Gradient Descent that we will use again and again when we study neural networks in [Part II](#): Batch GD, Mini-batch GD, and Stochastic GD.

Next we will look at Polynomial Regression, a more complex model that can fit non-linear datasets. Since this model has more parameters than Linear Regression, it is more prone to overfitting the training data, so we will look at how to detect whether or not this is the case, using learning curves, and then we will look at several regularization techniques that can reduce the risk of overfitting the training set.

Finally, we will look at two more models that are commonly used for classification tasks: Logistic Regression and Softmax Regression.



There will be quite a few math equations in this chapter, using basic notions of linear algebra and calculus. To understand these equations, you will need to know what vectors and matrices are, how to transpose them, what the dot product is, what matrix inverse is, and what partial derivatives are. If you are unfamiliar with these concepts, please go through the linear algebra and calculus introductory tutorials available as Jupyter notebooks in the online supplemental material. For those who are truly allergic to mathematics, you should still go through this chapter and simply skip the equations; hopefully, the text will be sufficient to help you understand most of the concepts.

Linear Regression

In [Chapter 1](#), we looked at a simple regression model of life satisfaction: $\text{life_satisfaction} = \theta_0 + \theta_1 \times \text{GDP_per_capita}$.

This model is just a linear function of the input feature `GDP_per_capita`. θ_0 and θ_1 are the model's parameters.

More generally, a linear model makes a prediction by simply computing a weighted sum of the input features, plus a constant called the *bias term* (also called the *intercept term*), as shown in [Equation 4-1](#).

Equation 4-1. Linear Regression model prediction

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

- \hat{y} is the predicted value.
- n is the number of features.
- x_i is the i^{th} feature value.
- θ_j is the j^{th} model parameter (including the bias term θ_0 and the feature weights $\theta_1, \theta_2, \dots, \theta_n$).

This can be written much more concisely using a vectorized form, as shown in [Equation 4-2](#).

Equation 4-2. Linear Regression model prediction (vectorized form)

$$\hat{y} = h_{\theta}(\mathbf{x}) = \theta^T \cdot \mathbf{x}$$

- θ is the model's *parameter vector*, containing the bias term θ_0 and the feature weights θ_1 to θ_n .
- θ^T is the transpose of θ (a row vector instead of a column vector).
- \mathbf{x} is the instance's *feature vector*, containing x_0 to x_n , with x_0 always equal to 1.
- $\theta^T \cdot \mathbf{x}$ is the dot product of θ^T and \mathbf{x} .
- h_{θ} is the hypothesis function, using the model parameters θ .

Okay, that's the Linear Regression model, so now how do we train it? Well, recall that training a model means setting its parameters so that the model best fits the training set. For this purpose, we first need a measure of how well (or poorly) the model fits the training data. In [Chapter 2](#) we saw that the most common performance measure of a regression model is the Root Mean Square Error (RMSE) ([Equation 2-1](#)). Therefore, to train a Linear Regression model, you need to find the value of θ that minimizes the RMSE. In practice, it is simpler to minimize the Mean Square Error (MSE) than the RMSE, and it leads to the same result (because the value that minimizes a function also minimizes its square root).¹

The MSE of a Linear Regression hypothesis h_{θ} on a training set \mathbf{X} is calculated using [Equation 4-3](#).

Equation 4-3. MSE cost function for a Linear Regression model

$$\text{MSE}(\mathbf{X}, h_{\theta}) = \frac{1}{m} \sum_{i=1}^m (\theta^T \cdot \mathbf{x}^{(i)} - y^{(i)})^2$$

Most of these notations were presented in [Chapter 2](#) (see “[Notations](#)” on page 38). The only difference is that we write h_{θ} instead of just h in order to make it clear that the model is parametrized by the vector θ . To simplify notations, we will just write $\text{MSE}(\theta)$ instead of $\text{MSE}(\mathbf{X}, h_{\theta})$.

¹ It is often the case that a learning algorithm will try to optimize a different function than the performance measure used to evaluate the final model. This is generally because that function is easier to compute, because it has useful differentiation properties that the performance measure lacks, or because we want to constrain the model during training, as we will see when we discuss regularization.

The Normal Equation

To find the value of θ that minimizes the cost function, there is a *closed-form solution* —in other words, a mathematical equation that gives the result directly. This is called the *Normal Equation* (Equation 4-4).²

Equation 4-4. Normal Equation

$$\hat{\theta} = (\mathbf{X}^T \cdot \mathbf{X})^{-1} \cdot \mathbf{X}^T \cdot \mathbf{y}$$

- $\hat{\theta}$ is the value of θ that minimizes the cost function.
- \mathbf{y} is the vector of target values containing $y^{(1)}$ to $y^{(m)}$.

Let's generate some linear-looking data to test this equation on (Figure 4-1):

```
import numpy as np

X = 2 * np.random.rand(100, 1)
y = 4 + 3 * X + np.random.randn(100, 1)
```

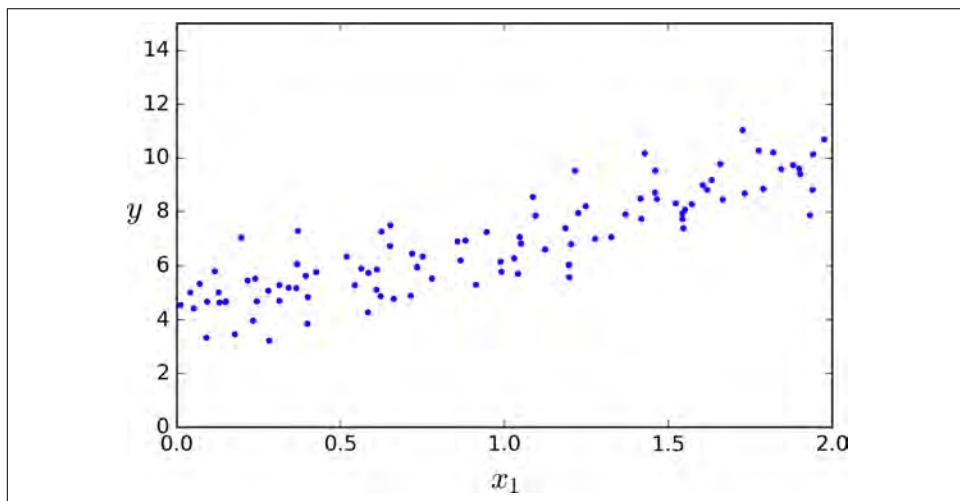


Figure 4-1. Randomly generated linear dataset

² The demonstration that this returns the value of θ that minimizes the cost function is outside the scope of this book.

Now let's compute $\hat{\theta}$ using the Normal Equation. We will use the `inv()` function from NumPy's Linear Algebra module (`np.linalg`) to compute the inverse of a matrix, and the `dot()` method for matrix multiplication:

```
X_b = np.c_[np.ones((100, 1)), X] # add x0 = 1 to each instance
theta_best = np.linalg.inv(X_b.T.dot(X_b)).dot(X_b.T).dot(y)
```

The actual function that we used to generate the data is $y = 4 + 3x_0 + \text{Gaussian noise}$. Let's see what the equation found:

```
>>> theta_best
array([[ 4.21509616],
       [ 2.77011339]])
```

We would have hoped for $\theta_0 = 4$ and $\theta_1 = 3$ instead of $\theta_0 = 3.865$ and $\theta_1 = 3.139$. Close enough, but the noise made it impossible to recover the exact parameters of the original function.

Now you can make predictions using $\hat{\theta}$:

```
>>> X_new = np.array([[0], [2]])
>>> X_new_b = np.c_[np.ones((2, 1)), X_new] # add x0 = 1 to each instance
>>> y_predict = X_new_b.dot(theta_best)
>>> y_predict
array([[ 4.21509616],
       [ 9.75532293]])
```

Let's plot this model's predictions (Figure 4-2):

```
plt.plot(X_new, y_predict, "r-")
plt.plot(X, y, "b.")
plt.axis([0, 2, 0, 15])
plt.show()
```

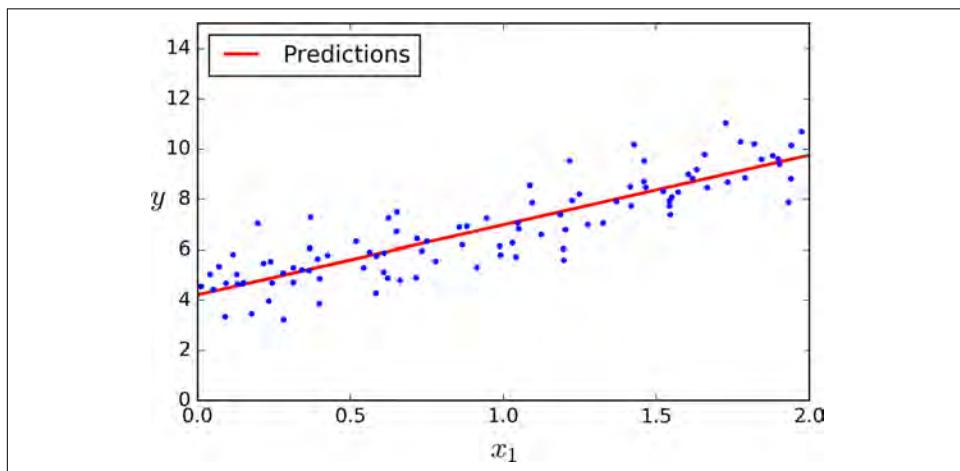


Figure 4-2. Linear Regression model predictions

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The equivalent code using Scikit-Learn looks like this:³

```
>>> from sklearn.linear_model import LinearRegression
>>> lin_reg = LinearRegression()
>>> lin_reg.fit(X, y)
>>> lin_reg.intercept_, lin_reg.coef_
(array([ 4.21509616]), array([[ 2.77011339]]))
>>> lin_reg.predict(X_new)
array([[ 4.21509616],
       [ 9.75532293]])
```

Computational Complexity

The Normal Equation computes the inverse of $\mathbf{X}^T \cdot \mathbf{X}$, which is an $n \times n$ matrix (where n is the number of features). The *computational complexity* of inverting such a matrix is typically about $O(n^{2.4})$ to $O(n^3)$ (depending on the implementation). In other words, if you double the number of features, you multiply the computation time by roughly $2^{2.4} = 5.3$ to $2^3 = 8$.



The Normal Equation gets very slow when the number of features grows large (e.g., 100,000).

On the positive side, this equation is linear with regards to the number of instances in the training set (it is $O(m)$), so it handles large training sets efficiently, provided they can fit in memory.

Also, once you have trained your Linear Regression model (using the Normal Equation or any other algorithm), predictions are very fast: the computational complexity is linear with regards to both the number of instances you want to make predictions on and the number of features. In other words, making predictions on twice as many instances (or twice as many features) will just take roughly twice as much time.

Now we will look at very different ways to train a Linear Regression model, better suited for cases where there are a large number of features, or too many training instances to fit in memory.

³ Note that Scikit-Learn separates the bias term (`intercept_`) from the feature weights (`coef_`).