CHAPTER 2

End-to-End Machine Learning Project

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In this chapter, you will go through an example project end to end, pretending to be a recently hired data scientist in a real estate company.[1] Here are the main steps you will go through:

1. Look at the big picture.
2. Get the data.
3. Discover and visualize the data to gain insights.
4. Prepare the data for Machine Learning algorithms.
5. Select a model and train it.
6. Fine-tune your model.
7. Present your solution.
8. Launch, monitor, and maintain your system.

1 The example project is completely fictitious; the goal is just to illustrate the main steps of a Machine Learning project, not to learn anything about the real estate business.

Working with Real Data

When you are learning about Machine Learning it is best to actually experiment with real-world data, not just artificial datasets. Fortunately, there are thousands of open datasets to choose from, ranging across all sorts of domains. Here are a few places you can look to get data:

- Popular open data repositories:
  - UC Irvine Machine Learning Repository
  - Kaggle datasets
  - Amazon's AWS datasets
- Meta portals (they list open data repositories):
  - *http://dataportals.org/*
  - *http://opendatamonitor.eu/*
  - *http://quandl.com/*
- Other pages listing many popular open data repositories:
  - Wikipedia's list of Machine Learning datasets
  - Quora.com question
  - Datasets subreddit

In this chapter we chose the California Housing Prices dataset from the StatLib repository[2] (see Figure 2-1). This dataset was based on data from the 1990 California census. It is not exactly recent (you could still afford a nice house in the Bay Area at the time), but it has many qualities for learning, so we will pretend it is recent data. We also added a categorical attribute and removed a few features for teaching purposes.

2 The original dataset appeared in R. Kelley Pace and Ronald Barry, "Sparse Spatial Autoregressions," *Statistics & Probability Letters* 33, no. 3 (1997): 291–297.

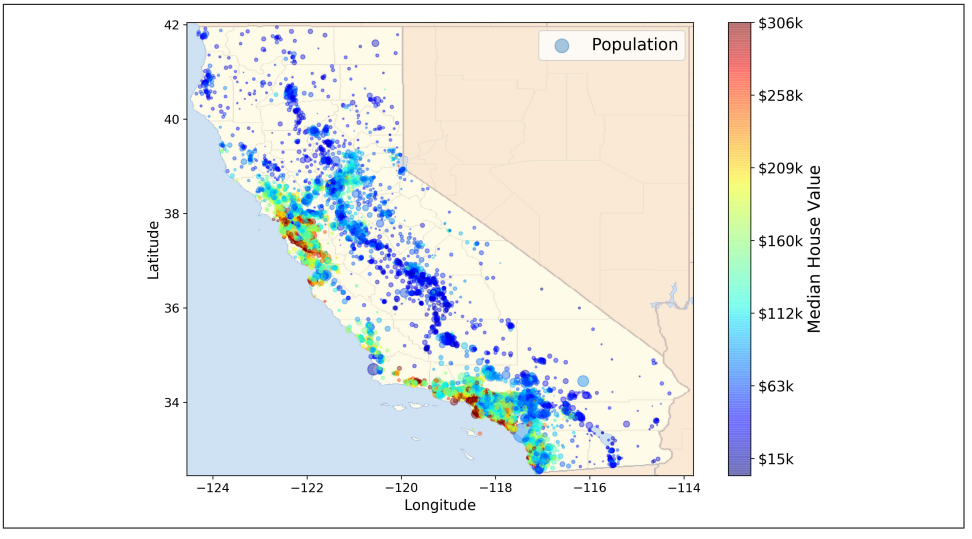

Figure 2-1. California housing prices

Look at the Big Picture

Welcome to Machine Learning Housing Corporation! The first task you are asked to perform is to build a model of housing prices in California using the California census data. This data has metrics such as the population, median income, median housing price, and so on for each block group in California. Block groups are the smallest geographical unit for which the US Census Bureau publishes sample data (a block group typically has a population of 600 to 3,000 people). We will just call them "districts" for short.

Your model should learn from this data and be able to predict the median housing price in any district, given all the other metrics.

Since you are a well-organized data scientist, the first thing you do is to pull out your Machine Learning project checklist. You can start with the one in ???; it should work reasonably well for most Machine Learning projects but make sure to adapt it to your needs. In this chapter we will go through many checklist items, but we will also skip a few, either because they are self-explanatory or because they will be discussed in later chapters.

Frame the Problem

The first question to ask your boss is what exactly is the business objective; building a model is probably not the end goal. How does the company expect to use and benefit

from this model? This is important because it will determine how you frame the problem, what algorithms you will select, what performance measure you will use to evaluate your model, and how much effort you should spend tweaking it.

Your boss answers that your model's output (a prediction of a district's median housing price) will be fed to another Machine Learning system (see Figure 2-2), along with many other *signals*.[3] This downstream system will determine whether it is worth investing in a given area or not. Getting this right is critical, as it directly affects revenue.

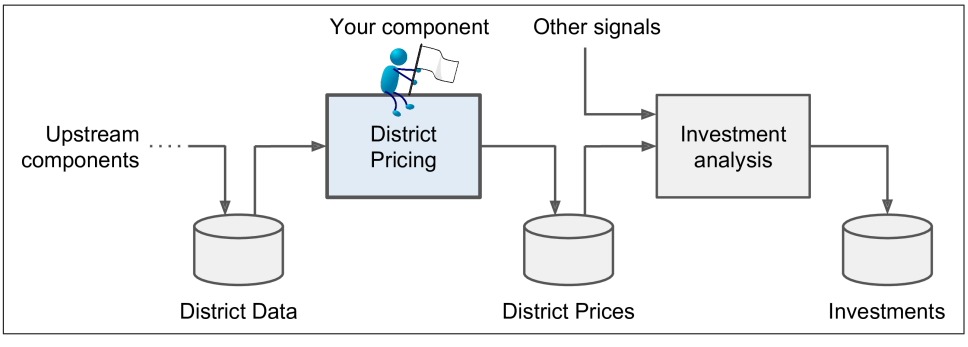

Figure 2-2. A Machine Learning pipeline for real estate investments

Pipelines

A sequence of data processing *components* is called a data *pipeline*. Pipelines are very common in Machine Learning systems, since there is a lot of data to manipulate and many data transformations to apply.

Components typically run asynchronously. Each component pulls in a large amount of data, processes it, and spits out the result in another data store, and then some time later the next component in the pipeline pulls this data and spits out its own output, and so on. Each component is fairly self-contained: the interface between components is simply the data store. This makes the system quite simple to grasp (with the help of a data flow graph), and different teams can focus on different components. Moreover, if a component breaks down, the downstream components can often continue to run normally (at least for a while) by just using the last output from the broken component. This makes the architecture quite robust.

3 A piece of information fed to a Machine Learning system is often called a *signal* in reference to Shannon's information theory: you want a high signal/noise ratio.

On the other hand, a broken component can go unnoticed for some time if proper monitoring is not implemented. The data gets stale and the overall system's performance drops.

The next question to ask is what the current solution looks like (if any). It will often give you a reference performance, as well as insights on how to solve the problem. Your boss answers that the district housing prices are currently estimated manually by experts: a team gathers up-to-date information about a district, and when they cannot get the median housing price, they estimate it using complex rules.

This is costly and time-consuming, and their estimates are not great; in cases where they manage to find out the actual median housing price, they often realize that their estimates were off by more than 20%. This is why the company thinks that it would be useful to train a model to predict a district's median housing price given other data about that district. The census data looks like a great dataset to exploit for this purpose, since it includes the median housing prices of thousands of districts, as well as other data.

Okay, with all this information you are now ready to start designing your system. First, you need to frame the problem: is it supervised, unsupervised, or Reinforcement Learning? Is it a classification task, a regression task, or something else? Should you use batch learning or online learning techniques? Before you read on, pause and try to answer these questions for yourself.

Have you found the answers? Let's see: it is clearly a typical supervised learning task since you are given *labeled* training examples (each instance comes with the expected output, i.e., the district's median housing price). Moreover, it is also a typical regression task, since you are asked to predict a value. More specifically, this is a *multiple regression* problem since the system will use multiple features to make a prediction (it will use the district's population, the median income, etc.). It is also a *univariate regression* problem since we are only trying to predict a single value for each district. If we were trying to predict multiple values per district, it would be a *multivariate regression* problem. Finally, there is no continuous flow of data coming in the system, there is no particular need to adjust to changing data rapidly, and the data is small enough to fit in memory, so plain batch learning should do just fine.

If the data was huge, you could either split your batch learning work across multiple servers (using the *MapReduce* technique), or you could use an online learning technique instead.

Select a Performance Measure

Your next step is to select a performance measure. A typical performance measure for regression problems is the Root Mean Square Error (RMSE). It gives an idea of how much error the system typically makes in its predictions, with a higher weight for large errors. Equation 2-1 shows the mathematical formula to compute the RMSE.

Equation 2-1. Root Mean Square Error (RMSE)

$$\text{RMSE}(\mathbf{X}, h) = \sqrt{\frac{1}{m}\sum_{i=1}^{m}\left(h\left(\mathbf{x}^{(i)}\right) - y^{(i)}\right)^2}$$

Notations

This equation introduces several very common Machine Learning notations that we will use throughout this book:

- m is the number of instances in the dataset you are measuring the RMSE on.
  - For example, if you are evaluating the RMSE on a validation set of 2,000 districts, then $m = 2{,}000$.
- $\mathbf{x}^{(i)}$ is a vector of all the feature values (excluding the label) of the i^{th} instance in the dataset, and $y^{(i)}$ is its label (the desired output value for that instance).
  - For example, if the first district in the dataset is located at longitude –118.29°, latitude 33.91°, and it has 1,416 inhabitants with a median income of $38,372, and the median house value is $156,400 (ignoring the other features for now), then:

$$\mathbf{x}^{(1)} = \begin{pmatrix} -118.29 \\ 33.91 \\ 1{,}416 \\ 38{,}372 \end{pmatrix}$$

  and:

$$y^{(1)} = 156{,}400$$

- $\mathbf{X}$ is a matrix containing all the feature values (excluding labels) of all instances in the dataset. There is one row per instance and the i^{th} row is equal to the transpose of $\mathbf{x}^{(i)}$, noted $(\mathbf{x}^{(i)})^T$.[4]
  - For example, if the first district is as just described, then the matrix $\mathbf{X}$ looks like this:

$$\mathbf{X} = \begin{pmatrix} \left(\mathbf{x}^{(1)}\right)^T \\ \left(\mathbf{x}^{(2)}\right)^T \\ \vdots \\ \left(\mathbf{x}^{(1999)}\right)^T \\ \left(\mathbf{x}^{(2000)}\right)^T \end{pmatrix} = \begin{pmatrix} -118.29 & 33.91 & 1{,}416 & 38{,}372 \\ \vdots & \vdots & \vdots & \vdots \end{pmatrix}$$

4 Recall that the transpose operator flips a column vector into a row vector (and vice versa).

- h is your system's prediction function, also called a *hypothesis*. When your system is given an instance's feature vector $\mathbf{x}^{(i)}$, it outputs a predicted value $\hat{y}^{(i)} = h(\mathbf{x}^{(i)})$ for that instance ($\hat{y}$ is pronounced "y-hat").
  - For example, if your system predicts that the median housing price in the first district is \$158,400, then $\hat{y}^{(1)} = h(\mathbf{x}^{(1)}) = 158{,}400$. The prediction error for this district is $\hat{y}^{(1)} - y^{(1)} = 2{,}000$.
- RMSE($\mathbf{X}$,h) is the cost function measured on the set of examples using your hypothesis h.

We use lowercase italic font for scalar values (such as m or $y^{(i)}$) and function names (such as h), lowercase bold font for vectors (such as $\mathbf{x}^{(i)}$), and uppercase bold font for matrices (such as $\mathbf{X}$).

Even though the RMSE is generally the preferred performance measure for regression tasks, in some contexts you may prefer to use another function. For example, suppose that there are many outlier districts. In that case, you may consider using the *Mean Absolute Error* (also called the Average Absolute Deviation; see Equation 2-2):

Equation 2-2. Mean Absolute Error

$$\text{MAE}(\mathbf{X}, h) = \frac{1}{m}\sum_{i=1}^{m}\left|h\left(\mathbf{x}^{(i)}\right) - y^{(i)}\right|$$

Both the RMSE and the MAE are ways to measure the distance between two vectors: the vector of predictions and the vector of target values. Various distance measures, or *norms*, are possible:

- Computing the root of a sum of squares (RMSE) corresponds to the *Euclidean norm*: it is the notion of distance you are familiar with. It is also called the ℓ_2 *norm*, noted $\|\cdot\|_2$ (or just $\|\cdot\|$).
- Computing the sum of absolutes (MAE) corresponds to the ℓ_1 *norm*, noted $\|\cdot\|_1$. It is sometimes called the *Manhattan norm* because it measures the distance between two points in a city if you can only travel along orthogonal city blocks.
- More generally, the ℓ_k *norm* of a vector $\mathbf{v}$ containing n elements is defined as $\|\mathbf{v}\|_k = \left(|v_0|^k + |v_1|^k + \cdots + |v_n|^k\right)^{\frac{1}{k}}$. ℓ_0 just gives the number of non-zero elements in the vector, and ℓ_∞ gives the maximum absolute value in the vector.
- The higher the norm index, the more it focuses on large values and neglects small ones. This is why the RMSE is more sensitive to outliers than the MAE. But when

outliers are exponentially rare (like in a bell-shaped curve), the RMSE performs very well and is generally preferred.

Check the Assumptions

Lastly, it is good practice to list and verify the assumptions that were made so far (by you or others); this can catch serious issues early on. For example, the district prices that your system outputs are going to be fed into a downstream Machine Learning system, and we assume that these prices are going to be used as such. But what if the downstream system actually converts the prices into categories (e.g., "cheap," "medium," or "expensive") and then uses those categories instead of the prices themselves? In this case, getting the price perfectly right is not important at all; your system just needs to get the category right. If that's so, then the problem should have been framed as a classification task, not a regression task. You don't want to find this out after working on a regression system for months.

Fortunately, after talking with the team in charge of the downstream system, you are confident that they do indeed need the actual prices, not just categories. Great! You're all set, the lights are green, and you can start coding now!

Get the Data

It's time to get your hands dirty. Don't hesitate to pick up your laptop and walk through the following code examples in a Jupyter notebook. The full Jupyter notebook is available at *https://github.com/ageron/handson-ml2*.

Create the Workspace

First you will need to have Python installed. It is probably already installed on your system. If not, you can get it at *https://www.python.org/*.[5]

Next you need to create a workspace directory for your Machine Learning code and datasets. Open a terminal and type the following commands (after the `$` prompts):

```
$ export ML_PATH="$HOME/ml"      # You can change the path if you prefer
$ mkdir -p $ML_PATH
```

You will need a number of Python modules: Jupyter, NumPy, Pandas, Matplotlib, and Scikit-Learn. If you already have Jupyter running with all these modules installed, you can safely skip to "Download the Data" on page 49. If you don't have them yet, there are many ways to install them (and their dependencies). You can use your sys-

5 The latest version of Python 3 is recommended. Python 2.7+ may work too, but it is now deprecated, all major scientific libraries are dropping support for it, so you should migrate to Python 3 as soon as possible.

tem's packaging system (e.g., apt-get on Ubuntu, or MacPorts or HomeBrew on MacOS), install a Scientific Python distribution such as Anaconda and use its packaging system, or just use Python's own packaging system, pip, which is included by default with the Python binary installers (since Python 2.7.9).[6] You can check to see if pip is installed by typing the following command:

```
$ python3 -m pip --version
pip 19.0.2 from [...]/lib/python3.6/site-packages (python 3.6)
```

You should make sure you have a recent version of pip installed. To upgrade the pip module, type:[7]

```
$ python3 -m pip install --user -U pip
Collecting pip
[...]
Successfully installed pip-19.0.2
```

Creating an Isolated Environment

If you would like to work in an isolated environment (which is strongly recommended so you can work on different projects without having conflicting library versions), install virtualenv[8] by running the following pip command (again, if you want virtualenv to be installed for all users on your machine, remove `--user` and run this command with administrator rights):

```
$ python3 -m pip install --user -U virtualenv
Collecting virtualenv
[...]
Successfully installed virtualenv
```

Now you can create an isolated Python environment by typing:

```
$ cd $ML_PATH
$ virtualenv env
Using base prefix '[...]'
New python executable in [...]/ml/env/bin/python3.6
Also creating executable in [...]/ml/env/bin/python
Installing setuptools, pip, wheel...done.
```

6 We will show the installation steps using pip in a bash shell on a Linux or MacOS system. You may need to adapt these commands to your own system. On Windows, we recommend installing Anaconda instead.

7 If you want to upgrade pip for all users on your machine rather than just your own user, you should remove the `--user` option and make sure you have administrator rights (e.g., by adding `sudo` before the whole command on Linux or MacOSX).

8 Alternative tools include venv (very similar to virtualenv and included in the standard library), virtualenvwrapper (provides extra functionalities on top of virtualenv), pyenv (allows easy switching between Python versions), and pipenv (a great packaging tool by the same author as the popular `requests` library, built on top of pip, virtualenv and more).

Now every time you want to activate this environment, just open a terminal and type:

```
$ cd $ML_PATH
$ source env/bin/activate # on Linux or MacOSX
$ .\env\Scripts\activate  # on Windows
```

To deactivate this environment, just type `deactivate`. While the environment is active, any package you install using pip will be installed in this isolated environment, and Python will only have access to these packages (if you also want access to the system's packages, you should create the environment using virtualenv's `--system-site-packages` option). Check out virtualenv's documentation for more information.

Now you can install all the required modules and their dependencies using this simple pip command (if you are not using a virtualenv, you will need the `--user` option or administrator rights):

```
$ python3 -m pip install -U jupyter matplotlib numpy pandas scipy scikit-learn
Collecting jupyter
  Downloading jupyter-1.0.0-py2.py3-none-any.whl
Collecting matplotlib
  [...]
```

To check your installation, try to import every module like this:

```
$ python3 -c "import jupyter, matplotlib, numpy, pandas, scipy, sklearn"
```

There should be no output and no error. Now you can fire up Jupyter by typing:

```
$ jupyter notebook
[I 15:24 NotebookApp] Serving notebooks from local directory: [...]/ml
[I 15:24 NotebookApp] 0 active kernels
[I 15:24 NotebookApp] The Jupyter Notebook is running at: http://localhost:8888/
[I 15:24 NotebookApp] Use Control-C to stop this server and shut down all
kernels (twice to skip confirmation).
```

A Jupyter server is now running in your terminal, listening to port 8888. You can visit this server by opening your web browser to *http://localhost:8888/* (this usually happens automatically when the server starts). You should see your empty workspace directory (containing only the *env* directory if you followed the preceding virtualenv instructions).

Now create a new Python notebook by clicking on the New button and selecting the appropriate Python version[9] (see Figure 2-3).

This does three things: first, it creates a new notebook file called *Untitled.ipynb* in your workspace; second, it starts a Jupyter Python kernel to run this notebook; and

9 Note that Jupyter can handle multiple versions of Python, and even many other languages such as R or Octave.

third, it opens this notebook in a new tab. You should start by renaming this notebook to "Housing" (this will automatically rename the file to *Housing.ipynb*) by clicking Untitled and typing the new name.

Figure 2-3. Your workspace in Jupyter

A notebook contains a list of cells. Each cell can contain executable code or formatted text. Right now the notebook contains only one empty code cell, labeled "In [1]:". Try typing **`print("Hello world!")`** in the cell, and click on the play button (see Figure 2-4) or press Shift-Enter. This sends the current cell to this notebook's Python kernel, which runs it and returns the output. The result is displayed below the cell, and since we reached the end of the notebook, a new cell is automatically created. Go through the User Interface Tour from Jupyter's Help menu to learn the basics.

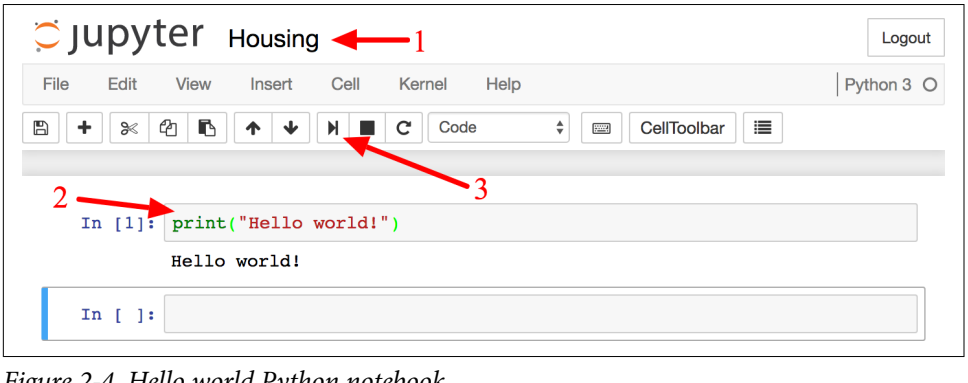

Figure 2-4. Hello world Python notebook