Machine Learning Lecture Notes

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1 Introduction to Probabilistic Modeling

Modeling the world around us and making predictions about the occurrence of events is a multidisciplinary endeavor standing on the solid foundations of probability theory, statistics, and computer science. Although intertwined in the process of modeling, these fields have relatively discernible roles and can be, to a degree, studied individually. Probability theory brings the mathematical infrastructure, firmly grounded in its axioms, for manipulating probabilities and equips us with a broad range of models with well-understood theoretical properties. Statistics contributes frameworks to formulate inference and the process of narrowing down the model space based on the observed data and our experience in order to find, and then analyze, solutions. Computer science provides us with theories, algorithms, and software to manage the data, compute the solutions, and study the relationship between solutions and available resources (time, space, computer architecture, etc.). As such, these three disciplines form the core quantitative framework for all of empirical science and beyond.

Probability theory and statistics have a relatively long history; the formal origins of both can be traced to the 17th century. Probability theory was developed out of efforts to understand games of chance and gambling. The correspondence between Blaise Pascal and Pierre de Fermat in 1654 serves as the oldest record of modern probability theory. Statistics, on the other hand, originated from data collection initiatives and attempts to understand trends in the society (e.g. manufacturing, mortality causes, value of land) and political affairs (e.g. public revenues, taxation, armies). The two disciplines started to merge in the 18th century with the use of data for inferential purposes in astronomy, geography, and social sciences. The increased complexity of models and availability of data in the 19th century emphasized the importance of computing machines. This contributed to establishing the foundations of the field of computer science in the 20th century, which is generally attributed to the introduction of the von Neumann architecture and formalization of the concept of an algorithm. The convergence of the three disciplines have reached the status of a principled theory of probabilistic inference with widespread applications in science, business, medicine, military, political campaigns, etc. Interestingly, various other disciplines have also contributed to the core techniques of probabilistic modeling.

Concepts such as Boltzmann distribution, genetic algorithm, or a neural network illustrate the influence of disciplines such as physics, biology, psychology, and engineering.

We will refer to the process of modeling, inference, and decision making based on probabilistic models as *reasoning under uncertainty*. Some form of reasoning under uncertainty is a necessary component of everyday life. When driving, for example, we often make decisions based on our expectations about which way would be best to take. While these situations do not usually involve an explicit use of probabilities and probabilistic models, an intelligent driverless car such as Google Chauffeur must make use of them. And so must a spam detection software in an email client, a credit card fraud detection system, or an algorithm that infers whether a particular genetic mutation will result in disease. Therefore, we first need to understand the concept of probability and then introduce a formal theory to incorporate evidence (e.g. data collected from instruments) in order to make good decisions in a range of situations. At a basic level, probabilities are used to quantify the chance of the occurrence of events. As Jacob Bernoulli brilliantly put it in his work *The Art of Conjecturing* (1713), "[p]robability, [...] is the degree of certainty, and it differs from the latter as a part differs from the whole". He later adds, "To make a conjecture [prediction] about something is the same as to measure its probability. Therefore, we define the art of conjecturing [science of prediction] or stochastics, as the art of measuring probabilities of things as accurately as possible, to the end that, in judgements and actions, we may always choose or follow that which has been found to be better, more satisfactory, safer, or more carefully considered." The techniques of probabilistic modeling formalize many intuitive concepts. In a nutshell, they provide toolkits for rigorous mathematical analysis and inference, often in the presence of evidence, about events influenced by factors that we either do not fully understand or have no control of.

To provide a quick insight into the concept of uncertainty and modeling, consider rolling a fair six-sided die. We could accurately predict, or so we think, the outcome of a roll if we carefully incorporated the initial position, force, friction, shape defects, and other physical factors and then executed the experiment. But the physical laws may not be known, they can be difficult to incorporate or such actions may not even be allowed by the rules of the experiment. Thus, it is practically useful to simply assume that each outcome is equally likely; in fact, if we rolled the die many times, we would indeed observe that each number is observed roughly equally. Assigning an equal chance (probability) to each outcome of the roll of a die provides an efficient and elegant way of modeling uncertainties inherent to the experiment.

Another, more realistic example in which collecting data provides a basis for simple probabilistic modeling is a situation of driving to work every day and predicting how long it will take us to reach the destination tomorrow. If we recorded the "time to work" for a few months we would observe that trips generally took different times depending on many internal (e.g. preferred speed for the day) and also external factors (e.g., weather, road works, encountering a slow driver). While these events, if known, could be used to predict the exact
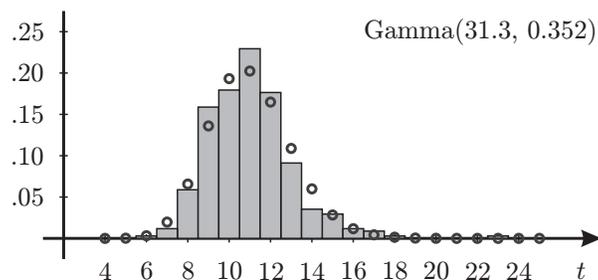
Figure 1: A histogram of recordings of the commute time (in minutes) to work. The data set contains 340 measurements collected over one year, for a distance of roughly 3.1 miles. The data was modeled using a gamma family of probability distributions, with the particular location and scale parameters estimated from the raw data. The values of the gamma distribution are shown as dark circles.

duration of the commute, it is unrealistic to expect to have full information. Therefore, it is useful to provide ways of aggregating external factors via collecting data over a period of time and providing the distribution of the commute time. Such a distribution, in the absence of any other information, would then facilitate reasoning about events such as making it on time to an important meeting at 9 am. One way of using the recorded data is to create histograms and calculate percentiles. Another would be to estimate the parameters of some mathematical function that fits the data well. Both approaches are illustrated in Figure 1.

As the examples above suggest, the techniques of probabilistic modeling provide a formalism for dealing with repetitive "experiments" influenced by a number of external factors over which we have little control or knowledge. However, we shall see later that probabilities need not be assigned only to events that repeat, but to any event in general. As long as they are assigned according to the formal axioms of probability, we can make inferences because the mathematical formalism does not depend on how the probabilities are assigned. This provides us an opportunity to incorporate our assumptions and existing knowledge into modeling, including the subjective assessments (beliefs) about occurrence of non-repetitive events. But let us start from the beginning.