1

Introduction

Two roads diverged in a wood, and I –
I took the one less traveled by,
And that has made all the difference.

Robert Frost, *The Road Not Taken*

1.1 Statistics and Machine Learning 🅰☺

Back in the early 1970s when the author was starting his undergraduate studies, freshmen interested in studying data analysis would pursue statistics in a mathematics department or a statistics department. In contrast, today's freshmen would most likely study machine learning in a computer science department, though they still have the option of majoring in statistics. Once there was one, now there are two options. Or is machine learning (ML) merely statistics with a fancy new wrapping? In this section, we will try to answer this question by first following the evolution of the two fields.

ML and statistics have very different origins, with statistics being the much older science. Statistics came from the German word *Statistik*, which appeared in 1749, meaning 'collection of data about the State', that is, government data on demographics and economics, useful for running the government. The collected data were analysed and the new science of *probability* was found to provide a solid mathematical foundation for data analysis. Probability itself began in 1654 when two famous French mathematicians, Blaise Pascal and Pierre de Fermat, solved a gambling problem brought to their attention by Antoine Gombaud. Christian Huygens wrote the first book on probability in 1657, followed by contributions from Jakob Bernoulli in 1713 and Abraham de Moivre in 1718. In 1812, Pierre de Laplace published *Théorie analytique des probabilités*, greatly expanding probability from games of chance to many scientific and practical

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problems. By the time of World War II, statistics was already a well-established field.

The birth of the electronic digital programmable computer by the end of World War II led to the growth of computer science and engineering, and the first successful numerical weather prediction in 1950 (Charney et al., 1950). While computers could compute with enormous speed and solve many problems, it soon became clear that they were very poor at performing simple tasks humans could do easily, such as recognizing a face, understanding speech, and so on.

The term *artificial intelligence* (AI) was invented by John McCarthy when he organized the Dartmouth Summer Research Project on Artificial Intelligence in 1956, an 8-week summer school held at Dartmouth College in Hanover, New Hampshire with about 20 invited attendees. This seminal workshop was considered by many to spark the field of AI research, with AI research mainly pursued by computer scientists/engineers and psychologists.

Machine learning (ML) is a major branch of AI[1] that allows computers to learn from data without being explicitly programmed. As for the origin of the term "machine learning", Turing (1950) raised the question 'can computers think?' and introduced the concept of "learning machines". In the 1955 Western Joint Computer Conference in Los Angeles, there was a session on "Learning Machines" (Nilsson, 2009), while the term 'machine learning' appeared later in Samuel (1959).

Meanwhile, the general public has become fascinated with the new genre of science fiction, depicting machines with human intelligence. Under this intoxicating atmosphere, some AI researchers became unrealistically optimistic about how soon it would take to produce intelligent machines; thus, a backlash against overpromises became inevitable. The UK Science Research Council asked the Cambridge Lucasian professor Sir James Lighthill to evaluate the academic research in AI with an outsider perspective, as Lighthill was a fluid dynamicist. The 1973 report was largely negative, stating that 'Most workers in AI research and in related fields confess to a pronounced feeling of disappointment in what has been achieved in the past twenty-five years. Workers entered the field around 1950, and even around 1960, with high hopes that are very far from having been realised in 1972. In no part of the field have the discoveries made so far produced the major impact that was then promised' (Lighthill, 1973). AI was devastated, as the UK closed all academic AI research except at three universities. Around the same time, the US Defense Advanced Research Projects Agency (then known as 'ARPA', now 'DARPA'), which had been the main source of AI funding in the US, also lost faith in AI, leading to drastic funding cuts. There were two major 'AI winters', periods of poor funding in AI, lasting around 1974–1980 and 1987–1993 (Crevier, 1993; Nilsson, 2009).

As AI suffered a tarnished reputation during the long AI winters, many researchers in AI in the mid-2000s referred to their work using other names, such as machine learning, informatics, computational intelligence, soft computing, data

[1] AI has other branches besides ML; for example *expert systems* were once very popular but have almost completely disappeared.

driven modelling, data mining and so on, partly to focus on a more specific aspect and partly to avoid the stigma of overpromises and science fiction overtones associated with the name 'artificial intelligence'. Google Trends reveals how terminology usage changes over time (see Fig. A1 in Appendix A), with 'machine learning' having been searched more often than 'artificial intelligence' on Google since 2015.

The general goal of having computers learning from data without being explicitly programmed was achieved in 1986 with an artificial neural network model called the multi-layer perceptron (Rumelhart et al., 1986a).[2] The rise of the Internet in the mid-1990s meant the connection of numerous computers and datasets, thereby introducing a huge amount of data for ML to extract useful information from. The commercial potential was quickly recognized, leading to the spectacular growth of many high technology companies, which in turn poured massive amounts of funding into ML and AI research.

By the late 1990s, statisticians introduced the new term '*data science*' to broaden statistics by including contributions by computer scientists (C. Hayashi, 1998; Cleveland, 2001). Data science is an interdisciplinary field that tries to extract knowledge from data using techniques from statistics, mathematics, computer science and information science. As such, one could consider statistics and ML as components within data science.

Did the separate paths of evolution taken by statistics and ML bring them to more or less the same domain within data science? Certainly there is partial overlap between the two, as it is not uncommon to have similar methods developed independently by statisticians and by ML scientists. Nevertheless, ML and statistics have their own distinct characteristics or cultures (Breiman, 2001b; D. R. Cox, Efron, et al., 2001). In fact, the two cultures are sufficiently different that it would be very difficult for ML to germinate from within statistics. For instance, one would expect counterculture art or music movements to germinate from societies with liberal laws rather with rigorous laws. Statistics, rooted in mathematics, requires a high standard in mathematical rigour for publications. While rigorous proofs can usually be derived for linear models, they may not even exist for the non-linear models used in ML. Thus, ML can only germinate within a culture that supports a more liberal, heuristic approach to research. Not surprisingly, ML germinated mainly from computer science, psychology, engineering and commerce.

When fitting a curve to a dataset, a statistician would ensure the number of adjustable model parameters is small compared to the sample size (that is, the number of observations) to avoid *overfitting*, that is, the model fitting to the noise in the data as the model becomes too flexible with abundant adjustable parameters (see Section 1.3). This prudent practice in statistics is not strictly followed in ML, as the number of parameters can be greater, sometimes much greater, than the sample size, as ML has developed ways to avoid overfitting while using a large number of parameters. The relatively large number of pa-

[2] While multi-layer perceptron neural network models became very popular after the appearance of Rumelhart et al. (1986a), there had been important contributions made by earlier researchers (Schmidhuber, 2015, section 5.5).

rameters renders ML models more difficult to interpret than statistical models; thus, ML models are often regarded somewhat dismissively as 'black boxes'.

The rationale of using large numbers of model parameters in ML is based on AI's desire to develop models following the architecture of the human brain. The following argument is attributed to Geoffrey Hinton, who often used it in his lectures: In the brain, there are more than 10^{14} synapses, that is, connections between nerve cells; thus, there are more than 10^{14} adjustable parameters in the brain. A human lifetime is of the order of 10^9 seconds, and learning say 10 data points per second implies a total sample size of 10^{10} in a lifetime. Thus, the number of parameters greatly exceeds the sample size for the human brain. In other words, if AI is to model the human brain function it has to explore the domain where the number of model parameters exceeds the sample size. For instance, in the ILSVRC-2012 image classification competition, the winning entry from Hinton's team used 60 million parameters trained with about 1.2 million images (Krizhevsky et al., 2012).

Dualism in nature was noted by the ancient Greek philosopher Heraclitus and in the Chinese philosophy of *yin and yang*, where opposite properties in nature may actually be complementary and interconnected and may give rise to each other as a wave trough gives rise to a wave crest. Yin is the shady or dark side and yang the sunny or bright side. Examples of traditional yin–yang pairs are night–day, moon–sun, feminine–masculine, soft–hard, and so on, and we can now add ML–statistics to the list as the yin and yang sides of data science (Fig. 1.1).

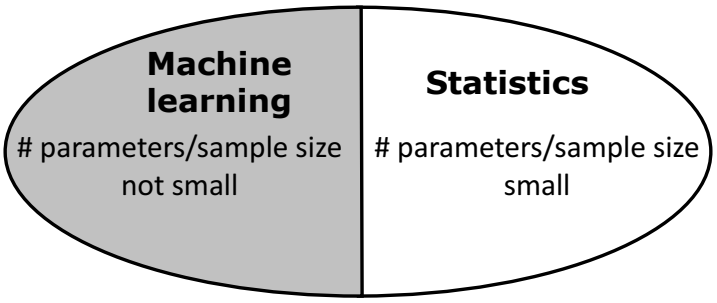

Figure 1.1 ML and statistics tend to occupy different parts of the data science space, as characterized by the number of model parameters to the sample size. In reality, there is overlap and more gradual transition between the two than the sharp boundary shown (see the Venn diagram in Fig. 15.1).

In journeys of discovery, the obscure yin side is often explored after the yang side. For instance, the European maritime exploration to India first proceeded eastward, and only westward from the time of Columbus, as sailing far into the obscure western ocean was not considered sensible nor profitable. In cosmology, the search had originally focused on visible, ordinary matter, but later it was

found that ordinary matter accounts for only 4.9% of the Universe, while the rest is the dark universe, containing dark matter (26.8%) and dark energy (68.3%) (Hodson, 2016). Similarly, in data science, the domain where the number of parameters is small relative to sample size was explored first by statisticians, and the seemingly meaningless domain of a large number of parameters was only explored much later by ML scientists, driven by their interest in building models that simulate the human brain. The old constraint requiring the number of parameters to be no larger than the sample size turned out to be breakable, much like the 'sound barrier' preventing supersonic flight. In Fig. 1.1, the yin and yang domains are drawn to be equal in size – in reality, the domain where the number of parameters is restricted to be small is much smaller than the domain without this restriction. The reason ML enjoyed much faster growth than statistics in recent decades is that the solutions of many problems in image and speech recognition, self-driving cars and so on lie in the domain of a large number of parameters.

Another major difference between the statistics and ML cultures lies in their treatment of predictor variables (Breiman, 2001b). Predictor selection, that is, choosing only the relevant predictor variables from a pool of predictors, is commonly practiced in statistics but not often in ML. ML generally does not consider throwing away information a good practice. Furthermore, first selecting predictors based on having high correlation with the response variable then building statistical/ML models leads to overestimation of the prediction skill (DelSole and Shukla, 2009).

In summary, the main tradeoff between statistics and ML is *interpretability* versus *accuracy*. With relatively few parameters and few predictors, statistical models are much more interpretable than ML models. For instance, the parameters in a linear regression model give useful information on how each predictor variable influences the response variable, whereas ML methods such as artificial neural networks and random forests are run as an ensemble of models initialized with different random numbers, leading to a huge number of parameters that are uninterpretable in practical problems. However, as datasets become increasingly larger and more complex, interpretability becomes harder and harder to achieve even with statistical models, while the advantage in prediction accuracy attained by ML models makes them increasingly attractive.

In physics, a similar transition occurred between classical mechanics and quantum mechanics in the 1920s. The clear deterministic view of classical mechanics was replaced by a fuzzy, random picture for atomic particles, thanks to revolutionary concepts like the Heisenberg uncertainty principle, wave-particle duality, and so on. Uncomfortable with the apparent randomness of nature in quantum mechanics, Einstein protested with the famous quote 'God does not play dice with the world' (Hermanns, 1983). A modern physicist learns both classical mechanics and quantum mechanics, using the former on everyday problems and the latter on atomic-scale problems. Similarly, a modern data scientist learns both statistics and machine learning, choosing the appropriate statistical or ML method based on the particular data problem.

1.2 Environmental Data Science 🅰☺

Environmental data science is the intersection between environmental science and data science. *Environmental science* (ES) is composed of many branches – atmospheric science, hydrology, oceanography, cryospheric science, ecology, agricultural science, remote sensing, climate science, environmental engineering, and so on, with the data from each branch having their own characteristics. Often, the plural term 'environmental sciences' is used to denote these branches. Statistical methods have long been popular in the environmental sciences, with numerous textbooks covering their applications in climate science (von Storch and Zwiers, 1999), atmospheric science (Wilks, 2011), oceanography (Thomson and Emery, 2014) and hydrology (Naghettini, 2007).

Environmental data tend to have different characteristics from non-environmental data. Most non-environmental datasets in ML applications contain *discrete data* (e.g. intensity of colour pixels in an image) and/or *categorical data* (e.g. alphabets and numbers in texts),[3] whereas most environmental datasets contain *continuous data* (e.g. temperature, air pressure, wind speed, precipitation amount, pollutant concentration, sea level, salinity, streamflow, crop yield, etc.). The discrete/categorical data from ML problems are in general bounded, that is, having a finite domain – for example, a colour pixel normally has intensity values ranging from 0 to 255, while texts are typically composed of 26 alphabets and 10 digits (plus upper cases and some special symbols). In contrast, continuous data are in general not bounded; for example, there are no guaranteed upper limits for variables such as wind speed, precipitation amount and pollutant concentration.

The most common data problem consists of predicting the value of an output variable (also known as a *response* variable or *dependent* variable) given the values of some input variables (a.k.a. *predictors* or *features*).[4] If the output variable is discrete or categorical, this is a *classification* problem, whereas if the output is continuous, it is a *regression* problem. Again, classification is much more common in non-environmental datasets, and many ML methods were developed first for classification and later modified for regression, such as support vector machines (Cortes and V. Vapnik, 1995; V. Vapnik et al., 1997).

After a model has been built or trained with a *training* dataset, its performance is usually evaluated with a separate *test* dataset. If the test input data lie outside the domain of the input data used to train the model, the model will be forced to do *extrapolation*, yielding inaccurate or even nonsensical predictions. Figure 1.2 illustrates why the outlier problem can be much worse with unbounded continuous input data than with finite-domain discrete/categorical data. Thus, making accurate predictions using environmental data could be a much harder problem than typical non-environmental data problems.

[3] The difference between categorical data (e.g. water, land, snow, ice) and discrete data (e.g. 1, 2, 3) is that categorical data normally have no natural ordering, though some categorical data (namely *ordinal data*) do have natural ordering (e.g. sunny, cloudy, rainy). See Section 2.1.

[4] "Predictors" are used in the statistics literature while "features" are used in ML.

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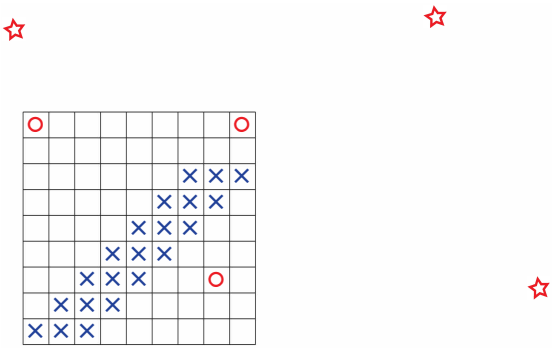

Figure 1.2 Schematic diagram illustrating the problem of outliers in the input data in 2-D. The grid illustrates a finite-domain discrete input data space with crosses indicating training data and circles marking outliers in the test data. For unbounded continuous input variables, the test data can lie well outside the grid and much farther from the training data, as illustrated by the stars.

Let us look at an example of input outliers. A common air quality measure of fine inhalable particles with diameters ≤ 2.5 μm is the $PM_{2.5}$ concentration. For predicting the hourly $PM_{2.5}$ concentration in Beijing, an important predictor is the cumulated precipitation (X. Liang et al., 2016), as the pollutant concentration drops after precipitation. When data from 2013 to 2015 were used for training non-linear regression models and data from 2010 to 2012 were used for testing, Hsieh (2020) noticed that the cumulated precipitation of an intense precipitation event reached 223.0 mm in the test data in July 2012, whereas the maximum value in the three years of training data was only 51.1 mm, that is, this input in the test data was over four times the maximum value in the training data, which led to wild extrapolation (Section 16.9).

From the old saying 'climate is what you expect; weather is what you get' (a similar version originated from Mark Twain), it follows that environmental problems also tend to group into 'weather' and 'climate' problems, with the former concerned with short-term variations and the latter concerned with the expected values from long-term records or with longer-term variations. For instance, by averaging daily weather data over three months, one obtains seasonal data and can build models to predict seasonal variations. Farmers, utility companies, and so on have great interest in seasonal forecasts, for example on whether next season will be warm or cool, dry or wet.

The averaging of weather data to form climate data changes the nature of the data through the central limit theorem from statistics. To illustrate this effect, consider the synthetic dataset

$$y = x + x^2 + \epsilon, \tag{1.1}$$

where x is a random variable obeying the Gaussian probability distribution with zero mean and unit standard deviation (see Section 3.4) and ϵ is Gaussian noise

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with a standard deviation of 0.5. Averaging these 'daily' data over 30 days reveals a dramatic weakening of the non-linear relation in the original daily data (Fig. 1.3). Thus, in this example, a non-linear regression model will greatly outperform a linear regression model in the daily data but not in the 30-day averaged data. In the real world, tomorrow's weather is not independent from today's weather (i.e. if it is rainy today, then tomorrow will also have higher odds of being rainy). Thus, the monthly data will be effectively averaging over far fewer than 30 independent observations as done in this synthetic dataset, so the weakening of the non-linear relation will not be as dramatic as in Fig. 1.3(c). Nevertheless, using non-linear regression models from ML on climate data will generally be less successful than using them on weather data due to the effects of the central limit theorem (Yuval and Hsieh, 2002).

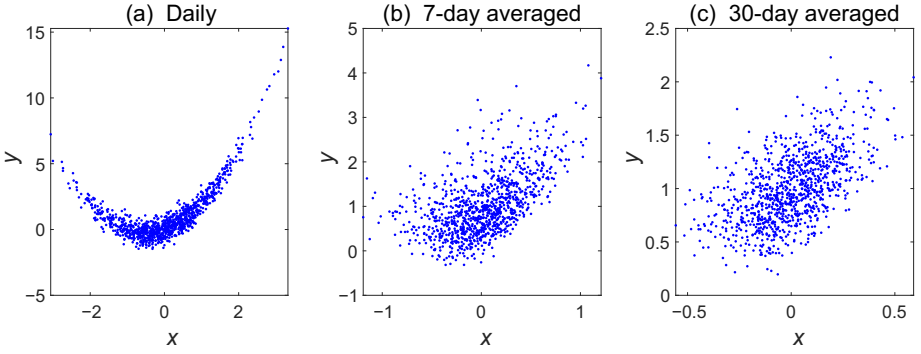

Figure 1.3 Effects of time-averaging on the non-linear relation (1.1). (a) Synthetic 'daily' data from a quadratic relation between x and y. The data time-averaged over (b) 7 observations and (c) 30 observations. [Follows Hsieh and Cannon (2008).]

Obtaining climate data from daily weather data by taking the time mean or average is no longer the only statistic used. In the last couple of decades, there has been a growing interest in the climate of extreme weather events (simply called 'climate extremes'), as global climate change may affect the extremes even more than the means. There is now a long list of such climate extreme variables derived from daily data, for example, the annual number of frost days, the maximum number of consecutive days when precipitation is < 1 mm, and so on (X. B. Zhang et al., 2011) and ML methods have been used to study climate extremes (Gaitan, Hsieh et al., 2014).

Like seeds broadly dispersed by the wind, ML models landing in numerous environmental fields germinated at different rates depending on the local conditions. If a field already had successful physics-based models, ML models tended to suffer from neglect and slow growth. Meteorology, where dynamical (a.k.a. numerical) models have been routinely used for weather forecasting, has been

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slower to embrace ML models than hydrology, where by the year 2000 there were already 43 hydrological papers using neural network models (Maier and Dandy, 2000). ML models were readily accepted in hydrology because physical-based hydrological models were not skillful in forecasting streamflow.[5] Remote sensing is another field where ML was quickly adopted (Benediktsson et al., 1990; Atkinson and Tatnall, 1997).

Compared to linear statistical models, non-linear ML models require larger sample sizes to excel. Oceanography, a field where collecting *in situ* observations is far more difficult than in meteorology or hydrology, and climate science, where the long timescales involved preclude large effective sample size, are fields where the adoption of ML have been relatively slow among the environmental sciences. Zwiers and Von Storch (2004) noted: 'much of the work that has had a large impact on climate research has used relatively simple techniques that allow transparent interpretation of the underlying physics'. Nevertheless, in the last few years, ML has grown rapidly even in fields such as oceanography and climate science. Perhaps even more unexpectedly, divergent approaches such as ML and physics have been merging in recent years within environmental science (Chapter 17). The history and practice of AI/ML in the environmental sciences have been reviewed by S. E. Haupt, Gagne et al. (2022) and Hsieh (2022).

1.3 A Simple Example of Curve Fitting 🅰☺

In this section, we will illustrate some basic concepts in data science by a simple example of curve fitting, using one independent variable x and one dependent variable y. Assume the true signal is a quadratic relation

$$y_{\text{signal}} = x - 0.25\, x^2. \tag{1.2}$$

The y data are composed of the signal plus random noise,

$$y = y_{\text{signal}} + \epsilon, \tag{1.3}$$

where the noise ϵ obeys a Gaussian probability distribution with zero mean and standard deviation being half that of y_{signal}. The advantage of using synthetic data in this example is that we know what the true signal is.

A polynomial of order m,

$$\hat{y} = w_0 + w_1 x + w_2 x^2 + \cdots + w_m x^m, \tag{1.4}$$

has $m + 1$ adjustable model parameters or weights w_j $(j = 0, ..., m)$, with $\hat{y}$ denoting the output value from the polynomial function as opposed to the value y from the data. Polynomials of order 1, 2, 4 and 9 are fitted to the training

[5] The difficulty lies in the subsurface flow passing through material, which is not easily observable. The subsurface flow is also complex and non-linear, thereby requiring many parameters to cover for the inexact physics, resulting also in poor model interpretability (Karpatne et al., 2017).

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dataset of 11 data points in Fig. 1.4 by minimizing the *mean squared error* (MSE) between the model output $\hat{y}$ and the data y,

$$\text{MSE} = \frac{1}{N}\sum_{i=1}^{N}(\hat{y}_i - y_i)^2, \tag{1.5}$$

where there are $i = 1, ..., N$ data points.

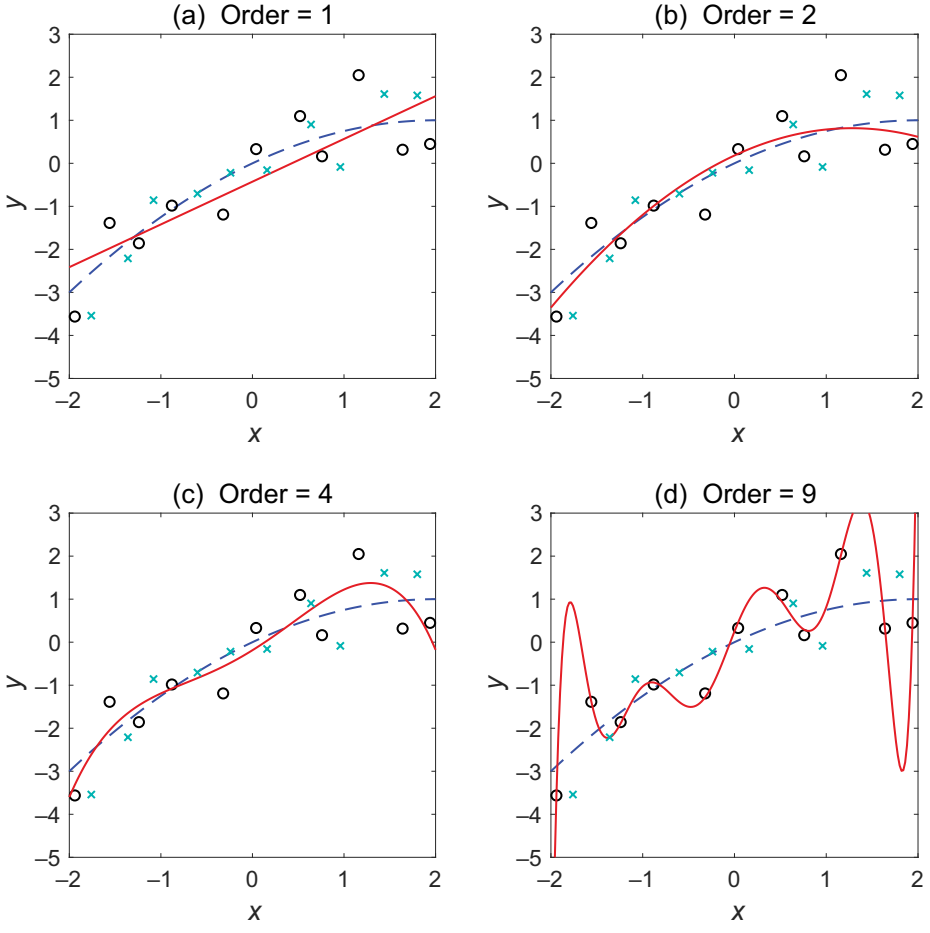

Figure 1.4 Polynomial fit to data using a polynomial of order (a) 1, (b) 2, (c) 4 and (d) 9. The circles indicate the 11 data points used for fitting (i.e. training), the solid curve the polynomial solution $\hat{y}$ and the dashed curve the true signal ($y_{\text{signal}} = x - 0.25\,x^2$). The crosses show 10 new data points used to validate the polynomial fit.

For order 1 (Fig. 1.4(a)), the polynomial reduces to a straight line and the problem is simple linear regression. As the order of the polynomial increases,

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the curve fit to the 11 training data points improves until the fit is almost perfect in Fig. 1.4(d), where the total number of adjustable parameters is 10, very close to the number of training data points. However, if one compares the polynomial fit (the solid curve) to the true signal (the dashed curve), while there is improvement going from order 1 to order 2, the agreement gets worse at order 4 and is dreadful at order 9.

This example illustrates the concepts of underfitting and overfitting data. At order 1, the model is *underfitting* the data since the true signal is a quadratic but the model is linear. However, as the order increases above 2, the model begins to *overfit* – that is, with more adjustable parameters than is needed to fit the true signal, the model is fitting to the noise in the data. An extra 10 new data points were generated from (1.2) and (1.3). The order 9 polynomial curve predicts these new data (marked by crosses) poorly (Fig. 1.4(d)), albeit the excellent fit to the training data (marked by circles).

With a real world problem, we will not have the luxury of knowing in advance what the true signal is and will be unable to know if our model is overfitting or underfitting. We need some independent *validation* data (sometimes also called test data) not used in the model training to tell us if the model is overfitting.[6] Figure 1.5 plots the mean squared error (MSE) for the training data and the validation data, as the order of the polynomial varies. The order 0 polynomial fit simply fits a constant to the training data, while the order 10 fit to the 11 data points is a perfect fit with zero MSE. While the MSE for the training data keeps dropping as the order increases, the MSE for the validation data drops to a minimum at order 2 then increases as the order increases. This tells us that the model was underfitting for order < 2 and overfitting for order > 2. Thus, we select the order 2 polynomial as the optimal model for this dataset. This process of using independent validation data to select the optimal model is called *model validation*.

What happens if we have more training data? Figures 1.6(a) and (b) compare the 9th order polynomial fit to training data with 15 and 100 points, respectively. The overfitting in (a) is much reduced in (b); thus, having more data helps in reducing overfitting.

What happens if the data are very noisy? In Fig. 1.6(c), the standard deviation of the added noise in y is four times that of Fig. 1.6(b), indicating noisier data make overfitting worse. However, if we increase the amount of noisy data to 1,000 points in Fig. 1.6(d), the overfitting is much reduced when compared with Fig. 1.6(c), where there are only 100 data points. Thus, one of the main reasons for success in modern data science is that even weak signals imbedded in very noisy data can be successful retrieved if massive amounts of data are available.

[6] Strictly speaking, training data, validation data and test data are all separate. Validation data are used to select the best model (e.g. the order 2 polynomial in our example). The performance of the selected model is then evaluated or verified with independent test data. Performance scores from test data are more trustworthy than those from the training and validation data, as the test data have not been used in model training and selection.

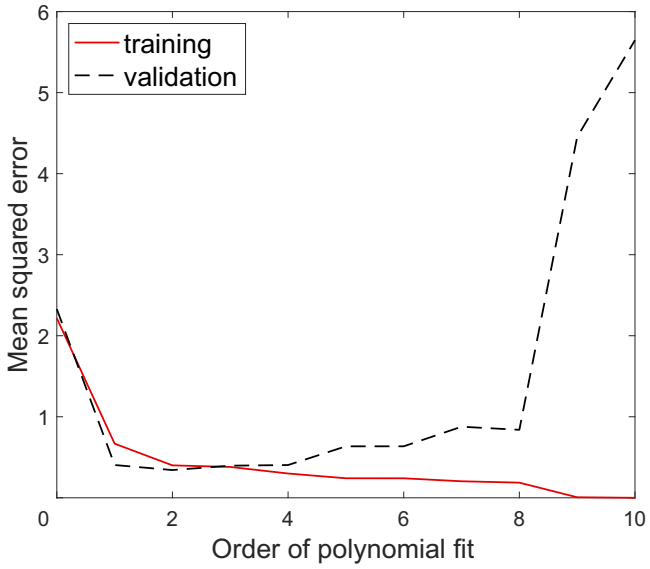

Figure 1.5 Mean squared error of the training and validation data as the order of the polynomial fit varies from 0 to 10.

What happens to the polynomial solution when we extend it outside the training data domain? Within the training domain of $x \in [-2, 2]$, the polynomial solutions for orders 2, 4 and 9 are quite similar to each other (Fig. 1.7), but when they extrapolate outside the training domain, the higher order solutions behave very badly. Furthermore, the wild extrapolation behaviour is irreproducible in that if we generate the synthetic data with a different initialization of the random number generator, we will get a different wild extrapolation picture in Fig. 1.7(d).

Polynomials are notorious for their extrapolation behaviour, since power functions of the form x^m $(m > 1)$ increase in magnitude much faster than x as $x \to \pm\infty$. Thus, modern data science methods such as artificial neural networks use basis functions with less aggressive growth properties than polynomials, which tame but still cannot rule out wild extrapolation (see Section 16.9).

1.4 Main Types of Data Problems 🅰☺

This section gives an overview on the basic types of data and data problems. Data are described by (a) discrete or categorical variables, (b) continuous variables and (c) probability distributions. Examples of discrete/categorical variables include binary variables (e.g. [0, 1], [on, off], [true, false]), [1, 2, 3], all integers and, in environmental science, [storm, no storm], [cold, warm], [cold, normal, warm], [dry, normal, wet], [land, water, snow, ice], and so on. Continuous variables in environmental science include temperature, wind speed,

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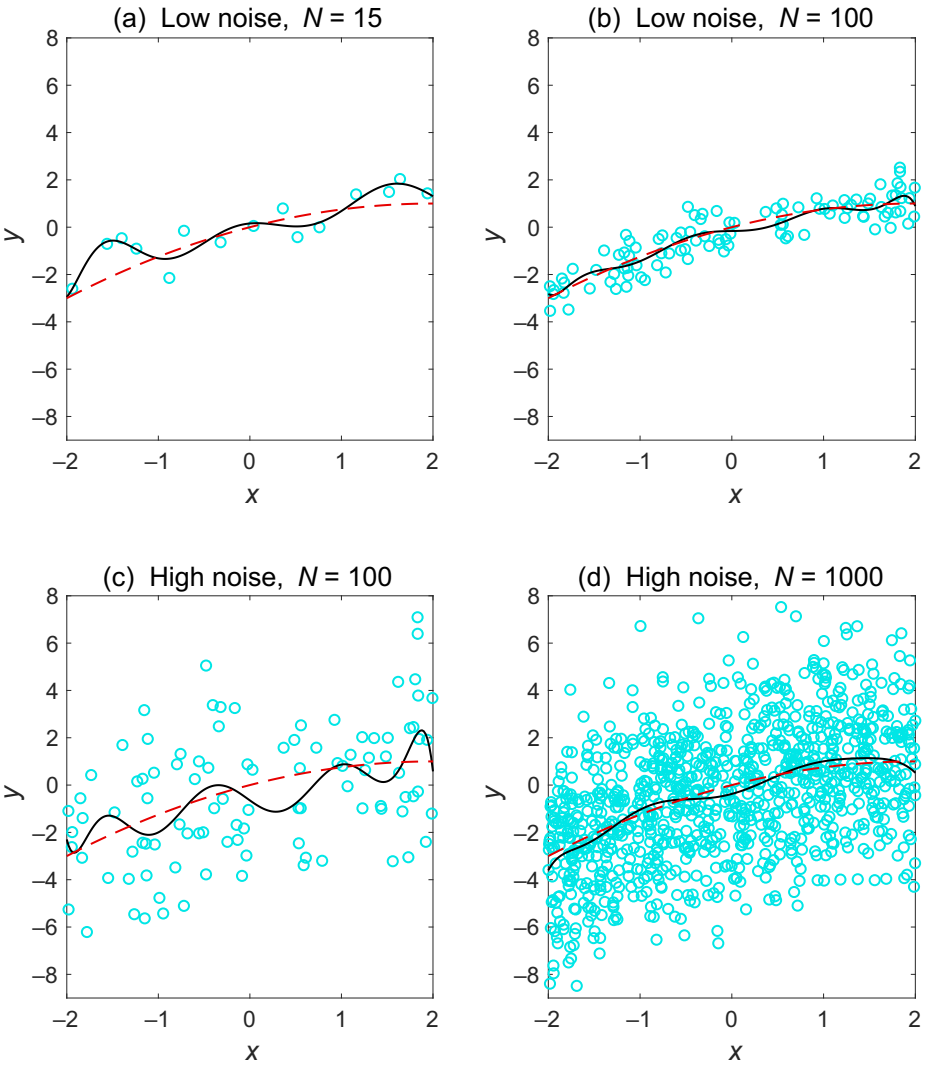

Figure 1.6 The ninth order polynomial fit to data with two noise levels and different numbers of training data points. The circles indicate the data points used for training, the solid curve the polynomial solution $\hat{y}$ and the dashed curve the true signal y_{signal}.

pollutant concentration, and so on. Examples of data described by probability distributions include a Gaussian distribution of given mean and standard deviation describing the temperature, a Weibull distribution describing the wind speed, and so on.

The early applications of ML were almost entirely done with discrete/categorical data; even today, the vast majority of ML applications in commercial

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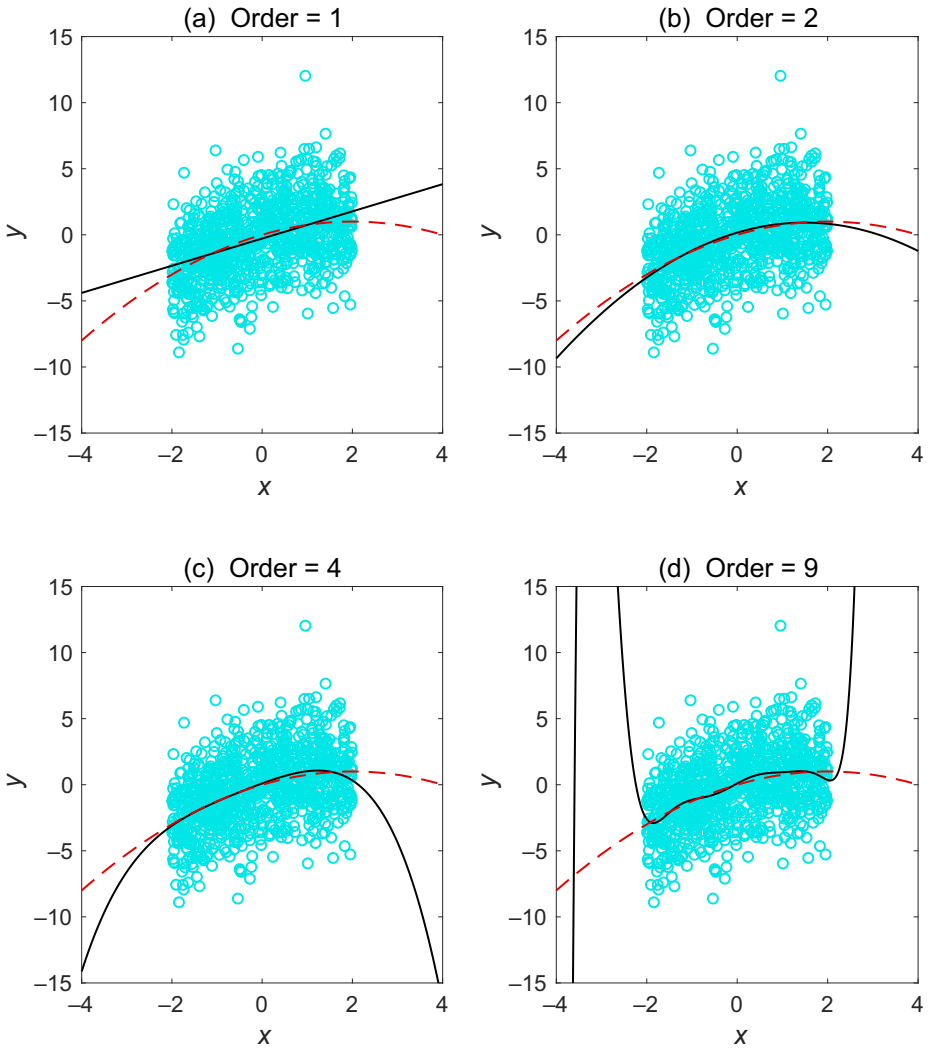

Figure 1.7 Extrapolating the polynomial solution to beyond the training data domain, where 1,000 data points (circles) were used for training and the order of the polynomial was (a) 1, (b) 2, (c) 4 and (d) 9. In (d), extending to the left side, the curve first shot up beyond the top of the plot, then plunged back down.

and engineering fields involve discrete/categorical data. In contrast, environmental scientists prefer continuous data, for example predicting tomorrow's temperature to be 28.4 °C instead of just being 'warm', which is rather vague. Statisticians prefer working with probability distributions, for example, the

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predicted temperature for tomorrow can be described by a Gaussian distribution with mean of 28.4 °C and a standard deviation of 1.6 °C. Of the three types of data description, the probability distribution approach contains the most information; however, it usually involves assuming the form of the distribution, for example Gaussian, which may or may not be a good assumption. With ML focusing on discrete/categorical data and statistics on probability distributions, there was very little linkage between ML and statistics in the early days. Fortunately, the linkage is much improved – for instance, most ML methods can now be cast in a probabilistic framework (K. P. Murphy, 2012).

What can we learn from the data? There are two main types of learning – *supervised learning* and *unsupervised learning*. An analogy for the former is a student trying to learn the correct French pronunciation being demonstrated by the teacher in a French class. An analogy for the latter is a solitary child playing with a jigsaw puzzle. In unsupervised learning, the student is provided with learning rules, but must rely on self-organization to arrive at a solution, without the benefit of being able to learn from a teacher's demonstration. Besides supervised and unsupervised learning, there is a third and less common type of learning – *reinforced learning*, which is briefly described in Section 1.4.3.

1.4.1 Supervised Learning 🅰☺

Given some training data $\{\mathbf{x}_i, \mathbf{y}_i\}$, $(i = 1, ..., N)$, supervised learning tries to find a mapping from the input variables $\mathbf{x}$ to the output variables $\hat{\mathbf{y}}$ (with the 'hat' on $\hat{\mathbf{y}}$ distinguishing the model output from the observed data or target data $\mathbf{y}_i$ or $\mathbf{y}$). For a new input $\mathbf{x}'$, one can then use the mapping to predict $\hat{\mathbf{y}}'$. The inputs are also called predictors, independent variables, features, attributes or covariates, and the outputs are also called response variables, dependent variables or predictands. N is called the sample size or the number of observations or data points. Observations are also called examples, cases or patterns in ML. In many applications, the model vector output $\hat{\mathbf{y}}$ reduces to a scalar $\hat{y}$.

Supervised learning is divided into *regression* and *classification* – regression if the output variables are real variables and classification if output variables are discrete/categorical. An example of regression: $\mathbf{x}$ contains three variables, air temperature, humidity and pressure, and $\hat{y}$ is the wind speed for the next day. For regression, the inputs are usually also real variables, though it is possible to include discrete/categorical variables in the inputs.

For classification, the discrete/categorical output $\hat{y} \in \{1, ..., C\}$, with C being the number of classes. If $C = 2$, this is binary classification, whereas for $C > 2$, multi-class classification. The inputs can be real or discrete/categorical variables. For instance, we can again have $\mathbf{x}$ containing air temperature, humidity and pressure, and $\hat{y}$ being 'storm' or 'no storm' for the next day – that is, the trained model will be used to issue storm warnings. Examples of multi-class classification include seasonal temperature forecasts of 'cool', 'normal' or 'warm' conditions, and satellite classifying observed ground pixels as being 'land', 'water', 'snow' or 'ice'.

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Environmental scientists may find it surprising that the non-environmental applications of ML are predominantly classification instead of regression. Examples of common non-environmental applications include: (i) spam filters classifying emails into 'spam' and 'not spam', (ii) banks classifying credit card transactions into 'suspicious' and 'not suspicious', (iii) handwriting recognition software using inputs of digitalized pixels of handwriting to classify into alphabets and numerals and (iv) object recognition software using inputs of photo images. In (iv), the number of classes can be very large, since the object in the photo can be a cat, rocket, car, house, and so on.

Some environmental problems involve both classification and regression, for example, in precipitation forecast, it is common to first use a classification model to choose between 'no precipitation' and 'precipitation', and if the output is 'precipitation', then a regression model is used to predict the amount of precipitation.

1.4.2 Unsupervised Learning 🅰☺

In contrast to supervised learning with input data $\mathbf{x}$ and output data $\hat{\mathbf{y}}$, unsupervised learning has only input data $\mathbf{x}$ to work with – the goal here is to find structure within the $\mathbf{x}$ data. For instance, some of the $\mathbf{x}$ data points are similar to each other and are located close together within the $\mathbf{x}$ space, so clustering is used to find the groups or clusters in the $\mathbf{x}$ data. For instance, the large-scale variability in the atmosphere displays several commonly occurring patterns (i.e. teleconnection patterns), and clustering (a.k.a. cluster analysis) (Section 10.1) has been used to extract these patterns from the atmospheric data (M. Bao and Wallace, 2015).

Another application involves reducing the $\mathbf{x}$ space. Suppose $\mathbf{x}$ contains 100 variables, spanning 100 dimensions. The data do not uniformly fill the 100-dimensional space, but may spread mainly along, say, two or three directions. Dimension reduction methods try to find the two or three directions displaying the strongest spread in the data. The essence of the 100-D dataset is now nicely condensed into a dataset with only two or three dimensions. For instance, principal component analysis (Chapter 9) (Jolliffe, 2002; Jolliffe and Cadima, 2016) is commonly used to condense high-dimensional environmental datasets to much lower dimensional datasets.

Which is more important – supervised or unsupervised learning? In Gorder (2006, p. 5), Professor Geoffrey Hinton was quoted on his view that human learning is mostly unsupervised:

> When we're learning to see, nobody's telling us what the right answers are – we just look. Every so often, your mother says "that's a dog", but that's very little information. You'd be lucky if you got a few bits of information – even one bit per second – that way. The brain's visual system requires 10^{14} [neural] connections. And you only live for 10^9 seconds. So it's no use learning one bit per second. You need more like 10^5 bits per second. And there's only one place you can get that much information – from the input itself.

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In their review of deep learning (i.e. neural network models with many processing layers), LeCun, Bengio, et al. (2015, p. 442) concluded:

> Unsupervised learning had a catalytic effect in reviving interest in deep learning, but has since been overshadowed by the successes of purely supervised learning ... we expect unsupervised learning to become far more important in the longer term. Human and animal learning is largely unsupervised: we discover the structure of the world by observing it, not by being told the name of every object.

1.4.3 Reinforced Learning A☺

Although much less widely used than supervised learning and unsupervised learning, reinforcement learning is still a notable branch of ML. Mainly used in game theory, control theory and operations research, reinforcement learning is concerned with improving the behaviour of intelligent agents (e.g. robots) to maximize the cumulative reward in an interactive environment. When training a robot soccer team, using supervised learning by teaching the robots to imitate the top human soccer players would be suboptimal, since the robots have different motor skills from humans (e.g. running speed, flexibility, balance, etc.). Instead, reinforced learning would use cumulative reward to gradually improve the performance of the robot soccer team. As the soccer team plays against other teams, rewards for good moves (e.g. controlling the ball, scoring a goal, etc.) and punishments for bad moves are used to gradually change the behaviour of the robots, so the team evolves into a stronger team (Riedmiller et al., 2009).

When building computer game players, using supervised learning by having the computer imitate the top human players would limit the skill of the computer player. To surpass the top human players, reinforced learning is needed. Reinforced learning using neural networks first became famous with the backgammon computer algorithm developed by Tesauro (1994), which improved its skills by playing against itself, eventually attaining the level of top human players.

Reinforced learning is not pursued in this book, as it does not appear to have important applications in the environmental sciences.

1.5 Curse of Dimensionality A☺

As modern datasets contain increasingly more variables, their high dimensions introduce a problem known as the 'curse of dimensionality' (Bellman, 1961), where data methods developed for low-dimensional datasets become unusable at high dimensions. Figure 1.8 illustrates the effect of increasing the dimension, where in 1-D, a segment of width 0.5 covers 1/2 of the unit interval [0, 1], in 2-D, a square of width 0.5 covers 1/4 of the unit square, while in 3-D, a cube of width 0.5 covers 1/8 of the unit cube. In a d-dimensional space, a hypercube of width 0.5 covers 2^{-d} of the unit hypercube. If one samples 100 data points over

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a hypercube, then in 1-D, each segment of width 0.5 will have an average of 50 data points, in 2-D each square of width 0.5 will have about 25 data points, and so on. In 10-D, there are $2^{10} = 1024$ hypercubes of width 0.5, so each hypercube contains less than 0.1 data point. In other words, sampling becomes very sparse for high-dimensional problems unless one has a huge amount of data. Techniques such as K-nearest neighbours (Section 12.4), which makes a prediction for a test input data by looking at the behaviour of its K nearest neighbours in the training data, break down at high dimension since the neighbours are far away. Thus, the problem of test input data being outliers relative to the training input data (as mentioned in Section 1.2) is more serious with high dimensions. The polynomial fit is another example of a method that generalizes poorly to high dimensions (Section 6.3.1).

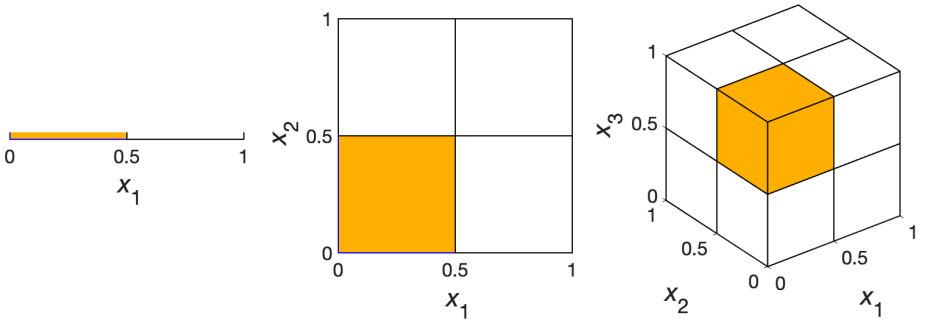

Figure 1.8 The 'curse of dimensionality' effect, as one proceeds from one to three dimensions.

In practice, methods have been successfully developed to work in high-dimensional space. Real high-dimensional data usually concentrate into a much smaller number of effective dimensions, and real data typically have some smoothness properties allowing local interpolation. Methods useful for high-dimensional problems tend to exploit these two properties.

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