$\boldsymbol{X}$ and $\boldsymbol{y}$, the cost function

$$J(\boldsymbol{w}, b) = -\mathbb{E}_{\mathbf{x},\mathrm{y}\sim\hat{p}_{\mathrm{data}}} \log p_{\mathrm{model}}(y \mid \boldsymbol{x}), \tag{5.100}$$

the model specification $p_{\mathrm{model}}(y \mid \boldsymbol{x}) = \mathcal{N}(y; \boldsymbol{x}^\top \boldsymbol{w} + b, 1)$, and, in most cases, the optimization algorithm defined by solving for where the gradient of the cost is zero using the normal equations.

By realizing that we can replace any of these components mostly independently from the others, we can obtain a very wide variety of algorithms.

The cost function typically includes at least one term that causes the learning process to perform statistical estimation. The most common cost function is the negative log-likelihood, so that minimizing the cost function causes maximum likelihood estimation.

The cost function may also include additional terms, such as regularization terms. For example, we can add weight decay to the linear regression cost function to obtain

$$J(\boldsymbol{w}, b) = \lambda ||\boldsymbol{w}||_2^2 - \mathbb{E}_{\mathbf{x},\mathrm{y}\sim\hat{p}_{\mathrm{data}}} \log p_{\mathrm{model}}(y \mid \boldsymbol{x}). \tag{5.101}$$

This still allows closed-form optimization.

If we change the model to be nonlinear, then most cost functions can no longer be optimized in closed form. This requires us to choose an iterative numerical optimization procedure, such as gradient descent.

The recipe for constructing a learning algorithm by combining models, costs, and optimization algorithms supports both supervised and unsupervised learning. The linear regression example shows how to support supervised learning. Unsupervised learning can be supported by defining a dataset that contains only $\boldsymbol{X}$ and providing an appropriate unsupervised cost and model. For example, we can obtain the first PCA vector by specifying that our loss function is

$$J(\boldsymbol{w}) = \mathbb{E}_{\mathbf{x}\sim\hat{p}_{\mathrm{data}}} ||\boldsymbol{x} - r(\boldsymbol{x}; \boldsymbol{w})||_2^2 \tag{5.102}$$

while our model is defined to have $\boldsymbol{w}$ with norm one and reconstruction function $r(\boldsymbol{x}) = \boldsymbol{w}^\top \boldsymbol{x} \boldsymbol{w}$.

In some cases, the cost function may be a function that we cannot actually evaluate, for computational reasons. In these cases, we can still approximately minimize it using iterative numerical optimization so long as we have some way of approximating its gradients.

Most machine learning algorithms make use of this recipe, though it may not immediately be obvious. If a machine learning algorithm seems especially unique or

hand-designed, it can usually be understood as using a special-case optimizer. Some models such as decision trees or k-means require special-case optimizers because their cost functions have flat regions that make them inappropriate for minimization by gradient-based optimizers. Recognizing that most machine learning algorithms can be described using this recipe helps to see the different algorithms as part of a taxonomy of methods for doing related tasks that work for similar reasons, rather than as a long list of algorithms that each have separate justifications.

5.11 Challenges Motivating Deep Learning

The simple machine learning algorithms described in this chapter work very well on a wide variety of important problems. However, they have not succeeded in solving the central problems in AI, such as recognizing speech or recognizing objects.

The development of deep learning was motivated in part by the failure of traditional algorithms to generalize well on such AI tasks.

This section is about how the challenge of generalizing to new examples becomes exponentially more difficult when working with high-dimensional data, and how the mechanisms used to achieve generalization in traditional machine learning are insufficient to learn complicated functions in high-dimensional spaces. Such spaces also often impose high computational costs. Deep learning was designed to overcome these and other obstacles.

5.11.1 The Curse of Dimensionality

Many machine learning problems become exceedingly difficult when the number of dimensions in the data is high. This phenomenon is known as the **curse of dimensionality**. Of particular concern is that the number of possible distinct configurations of a set of variables increases exponentially as the number of variables increases.

Figure 5.9: As the number of relevant dimensions of the data increases (from left to right), the number of configurations of interest may grow exponentially. *(Left)*In this one-dimensional example, we have one variable for which we only care to distinguish 10 regions of interest. With enough examples falling within each of these regions (each region corresponds to a cell in the illustration), learning algorithms can easily generalize correctly. A straightforward way to generalize is to estimate the value of the target function within each region (and possibly interpolate between neighboring regions). *(Center)*With 2 dimensions it is more difficult to distinguish 10 different values of each variable. We need to keep track of up to 10×10=100 regions, and we need at least that many examples to cover all those regions. *(Right)*With 3 dimensions this grows to $10^3 = 1000$ regions and at least that many examples. For d dimensions and v values to be distinguished along each axis, we seem to need $O(v^d)$ regions and examples. This is an instance of the curse of dimensionality. Figure graciously provided by Nicolas Chapados.

The curse of dimensionality arises in many places in computer science, and especially so in machine learning.

One challenge posed by the curse of dimensionality is a statistical challenge. As illustrated in figure 5.9, a statistical challenge arises because the number of possible configurations of $\boldsymbol{x}$ is much larger than the number of training examples. To understand the issue, let us consider that the input space is organized into a grid, like in the figure. We can describe low-dimensional space with a low number of grid cells that are mostly occupied by the data. When generalizing to a new data point, we can usually tell what to do simply by inspecting the training examples that lie in the same cell as the new input. For example, if estimating the probability density at some point $\boldsymbol{x}$, we can just return the number of training examples in the same unit volume cell as $\boldsymbol{x}$, divided by the total number of training examples. If we wish to classify an example, we can return the most common class of training examples in the same cell. If we are doing regression we can average the target values observed over the examples in that cell. But what about the cells for which we have seen no example? Because in high-dimensional spaces the number of configurations is huge, much larger than our number of examples, a typical grid cell has no training example associated with it. How could we possibly say something

meaningful about these new configurations? Many traditional machine learning algorithms simply assume that the output at a new point should be approximately the same as the output at the nearest training point.

5.11.2 Local Constancy and Smoothness Regularization

In order to generalize well, machine learning algorithms need to be guided by prior beliefs about what kind of function they should learn. Previously, we have seen these priors incorporated as explicit beliefs in the form of probability distributions over parameters of the model. More informally, we may also discuss prior beliefs as directly influencing the *function* itself and only indirectly acting on the parameters via their effect on the function. Additionally, we informally discuss prior beliefs as being expressed implicitly, by choosing algorithms that are biased toward choosing some class of functions over another, even though these biases may not be expressed (or even possible to express) in terms of a probability distribution representing our degree of belief in various functions.

Among the most widely used of these implicit "priors" is the **smoothness prior** or **local constancy prior**. This prior states that the function we learn should not change very much within a small region.

Many simpler algorithms rely exclusively on this prior to generalize well, and as a result they fail to scale to the statistical challenges involved in solving AI-level tasks. Throughout this book, we will describe how deep learning introduces additional (explicit and implicit) priors in order to reduce the generalization error on sophisticated tasks. Here, we explain why the smoothness prior alone is insufficient for these tasks.

There are many different ways to implicitly or explicitly express a prior belief that the learned function should be smooth or locally constant. All of these different methods are designed to encourage the learning process to learn a function f^* that satisfies the condition

$$f^*(\boldsymbol{x}) \approx f^*(\boldsymbol{x} + \epsilon) \tag{5.103}$$

for most configurations $\boldsymbol{x}$ and small change ϵ. In other words, if we know a good answer for an input $\boldsymbol{x}$ (for example, if $\boldsymbol{x}$ is a labeled training example) then that answer is probably good in the neighborhood of $\boldsymbol{x}$. If we have several good answers in some neighborhood we would combine them (by some form of averaging or interpolation) to produce an answer that agrees with as many of them as much as possible.

An extreme example of the local constancy approach is the k-nearest neighbors family of learning algorithms. These predictors are literally constant over each

region containing all the points $\boldsymbol{x}$ that have the same set of k nearest neighbors in the training set. For $k = 1$, the number of distinguishable regions cannot be more than the number of training examples.

While the k-nearest neighbors algorithm copies the output from nearby training examples, most kernel machines interpolate between training set outputs associated with nearby training examples. An important class of kernels is the family of **local kernels** where $k(\boldsymbol{u}, \boldsymbol{v})$ is large when $\boldsymbol{u} = \boldsymbol{v}$ and decreases as $\boldsymbol{u}$ and $\boldsymbol{v}$ grow farther apart from each other. A local kernel can be thought of as a similarity function that performs template matching, by measuring how closely a test example $\boldsymbol{x}$ resembles each training example $\boldsymbol{x}^{(i)}$. Much of the modern motivation for deep learning is derived from studying the limitations of local template matching and how deep models are able to succeed in cases where local template matching fails (Bengio *et al.*, 2006b).

Decision trees also suffer from the limitations of exclusively smoothness-based learning because they break the input space into as many regions as there are leaves and use a separate parameter (or sometimes many parameters for extensions of decision trees) in each region. If the target function requires a tree with at least n leaves to be represented accurately, then at least n training examples are required to fit the tree. A multiple of n is needed to achieve some level of statistical confidence in the predicted output.

In general, to distinguish $O(k)$ regions in input space, all of these methods require $O(k)$ examples. Typically there are $O(k)$ parameters, with $O(1)$ parameters associated with each of the $O(k)$ regions. The case of a nearest neighbor scenario, where each training example can be used to define at most one region, is illustrated in figure 5.10.

Is there a way to represent a complex function that has many more regions to be distinguished than the number of training examples? Clearly, assuming only smoothness of the underlying function will not allow a learner to do that. For example, imagine that the target function is a kind of checkerboard. A checkerboard contains many variations but there is a simple structure to them. Imagine what happens when the number of training examples is substantially smaller than the number of black and white squares on the checkerboard. Based on only local generalization and the smoothness or local constancy prior, we would be guaranteed to correctly guess the color of a new point if it lies within the same checkerboard square as a training example. There is no guarantee that the learner could correctly extend the checkerboard pattern to points lying in squares that do not contain training examples. With this prior alone, the only information that an example tells us is the color of its square, and the only way to get the colors of the

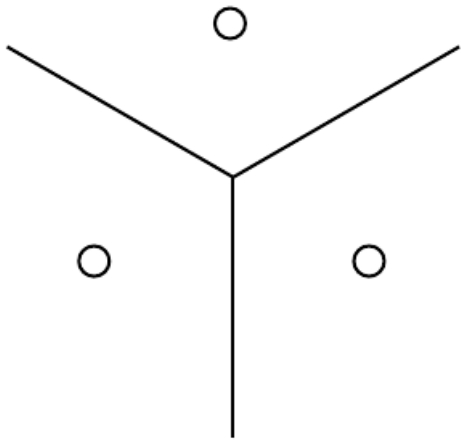

Figure 5.10: Illustration of how the nearest neighbor algorithm breaks up the input space into regions. An example (represented here by a circle) within each region defines the region boundary (represented here by the lines). The y value associated with each example defines what the output should be for all points within the corresponding region. The regions defined by nearest neighbor matching form a geometric pattern called a Voronoi diagram. The number of these contiguous regions cannot grow faster than the number of training examples. While this figure illustrates the behavior of the nearest neighbor algorithm specifically, other machine learning algorithms that rely exclusively on the local smoothness prior for generalization exhibit similar behaviors: each training example only informs the learner about how to generalize in some neighborhood immediately surrounding that example.

entire checkerboard right is to cover each of its cells with at least one example.

The smoothness assumption and the associated non-parametric learning algorithms work extremely well so long as there are enough examples for the learning algorithm to observe high points on most peaks and low points on most valleys of the true underlying function to be learned. This is generally true when the function to be learned is smooth enough and varies in few enough dimensions. In high dimensions, even a very smooth function can change smoothly but in a different way along each dimension. If the function additionally behaves differently in different regions, it can become extremely complicated to describe with a set of training examples. If the function is complicated (we want to distinguish a huge number of regions compared to the number of examples), is there any hope to generalize well?

The answer to both of these questions—whether it is possible to represent a complicated function efficiently, and whether it is possible for the estimated function to generalize well to new inputs—is yes. The key insight is that a very large number of regions, e.g., $O(2^k)$, can be defined with $O(k)$ examples, so long as we introduce some dependencies between the regions via additional assumptions about the underlying data generating distribution. In this way, we can actually generalize non-locally (Bengio and Monperrus, 2005; Bengio *et al.*, 2006c). Many different deep learning algorithms provide implicit or explicit assumptions that are reasonable for a broad range of AI tasks in order to capture these advantages.

Other approaches to machine learning often make stronger, task-specific assumptions. For example, we could easily solve the checkerboard task by providing the assumption that the target function is periodic. Usually we do not include such strong, task-specific assumptions into neural networks so that they can generalize to a much wider variety of structures. AI tasks have structure that is much too complex to be limited to simple, manually specified properties such as periodicity, so we want learning algorithms that embody more general-purpose assumptions. The core idea in deep learning is that we assume that the data was generated by the *composition of factors* or features, potentially at multiple levels in a hierarchy. Many other similarly generic assumptions can further improve deep learning algorithms. These apparently mild assumptions allow an exponential gain in the relationship between the number of examples and the number of regions that can be distinguished. These exponential gains are described more precisely in sections 6.4.1, 15.4 and 15.5. The exponential advantages conferred by the use of deep, distributed representations counter the exponential challenges posed by the curse of dimensionality.

5.11.3 Manifold Learning

An important concept underlying many ideas in machine learning is that of a manifold.

A **manifold** is a connected region. Mathematically, it is a set of points, associated with a neighborhood around each point. From any given point, the manifold locally appears to be a Euclidean space. In everyday life, we experience the surface of the world as a 2-D plane, but it is in fact a spherical manifold in 3-D space.

The definition of a neighborhood surrounding each point implies the existence of transformations that can be applied to move on the manifold from one position to a neighboring one. In the example of the world's surface as a manifold, one can walk north, south, east, or west.

Although there is a formal mathematical meaning to the term "manifold," in machine learning it tends to be used more loosely to designate a connected set of points that can be approximated well by considering only a small number of degrees of freedom, or dimensions, embedded in a higher-dimensional space. Each dimension corresponds to a local direction of variation. See figure 5.11 for an example of training data lying near a one-dimensional manifold embedded in two-dimensional space. In the context of machine learning, we allow the dimensionality of the manifold to vary from one point to another. This often happens when a manifold intersects itself. For example, a figure eight is a manifold that has a single dimension in most places but two dimensions at the intersection at the center.

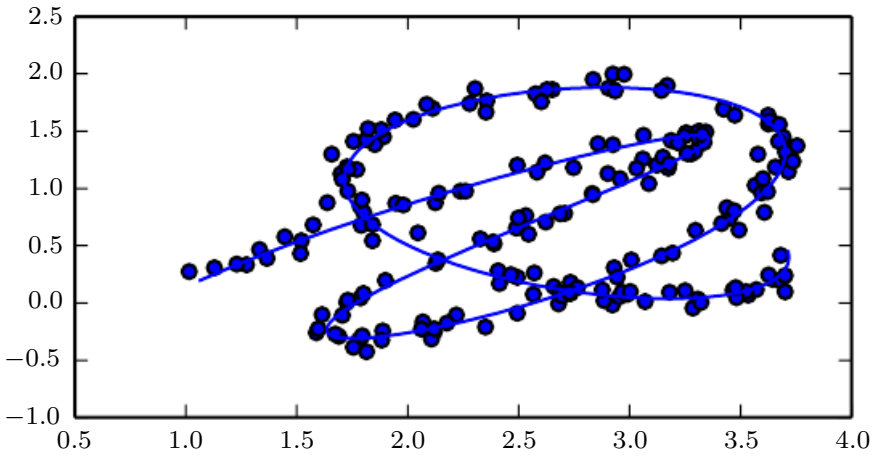

Figure 5.11: Data sampled from a distribution in a two-dimensional space that is actually concentrated near a one-dimensional manifold, like a twisted string. The solid line indicates the underlying manifold that the learner should infer.

Many machine learning problems seem hopeless if we expect the machine learning algorithm to learn functions with interesting variations across all of $\mathbb{R}^n$. **Manifold learning** algorithms surmount this obstacle by assuming that most of $\mathbb{R}^n$ consists of invalid inputs, and that interesting inputs occur only along a collection of manifolds containing a small subset of points, with interesting variations in the output of the learned function occurring only along directions that lie on the manifold, or with interesting variations happening only when we move from one manifold to another. Manifold learning was introduced in the case of continuous-valued data and the unsupervised learning setting, although this probability concentration idea can be generalized to both discrete data and the supervised learning setting: the key assumption remains that probability mass is highly concentrated.

The assumption that the data lies along a low-dimensional manifold may not always be correct or useful. We argue that in the context of AI tasks, such as those that involve processing images, sounds, or text, the manifold assumption is at least approximately correct. The evidence in favor of this assumption consists of two categories of observations.

The first observation in favor of the **manifold hypothesis** is that the probability distribution over images, text strings, and sounds that occur in real life is highly concentrated. Uniform noise essentially never resembles structured inputs from these domains. Figure 5.12 shows how, instead, uniformly sampled points look like the patterns of static that appear on analog television sets when no signal is available. Similarly, if you generate a document by picking letters uniformly at random, what is the probability that you will get a meaningful English-language text? Almost zero, again, because most of the long sequences of letters do not correspond to a natural language sequence: the distribution of natural language sequences occupies a very small volume in the total space of sequences of letters.

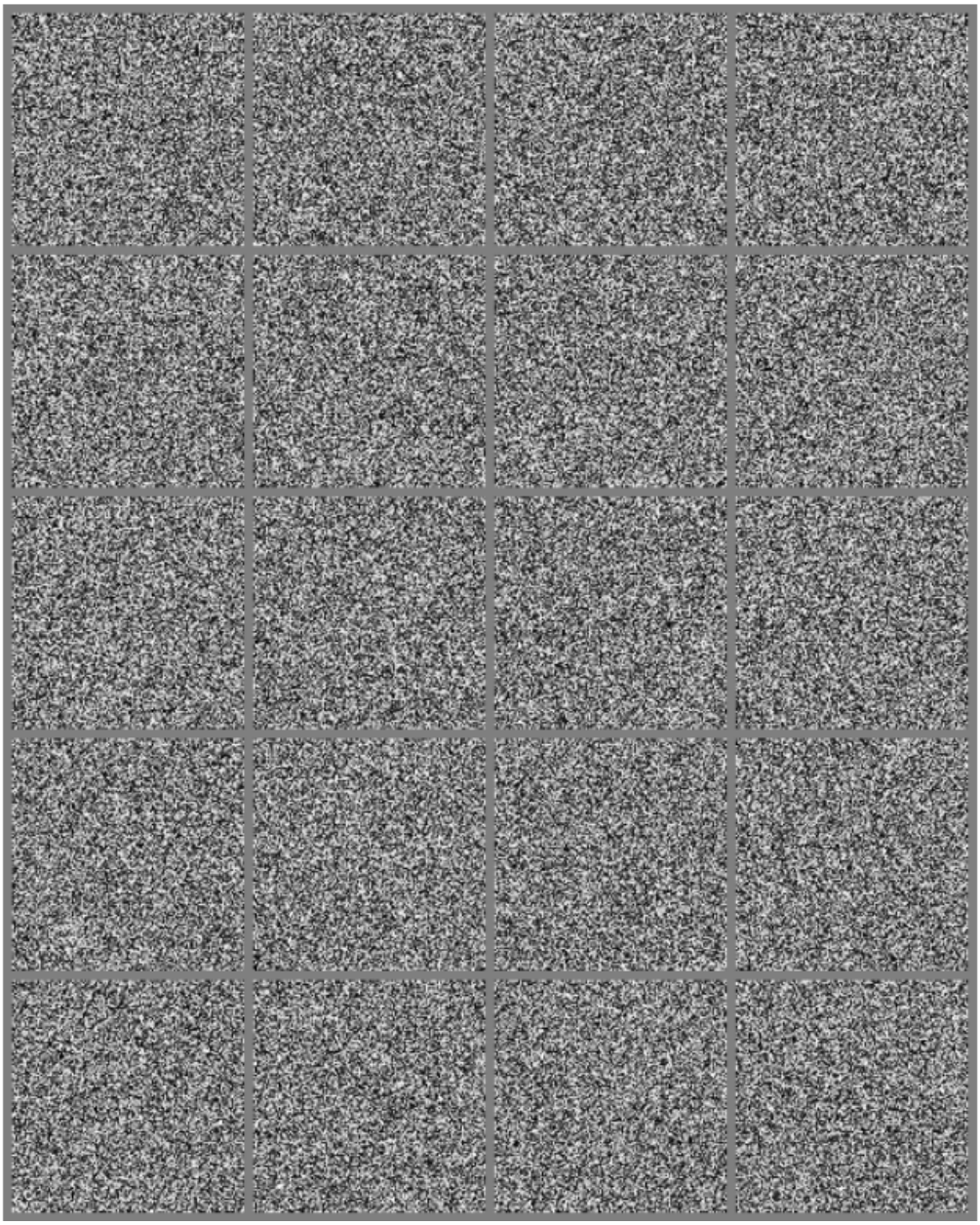

Figure 5.12: Sampling images uniformly at random (by randomly picking each pixel according to a uniform distribution) gives rise to noisy images. Although there is a non-zero probability to generate an image of a face or any other object frequently encountered in AI applications, we never actually observe this happening in practice. This suggests that the images encountered in AI applications occupy a negligible proportion of the volume of image space.

Of course, concentrated probability distributions are not sufficient to show that the data lies on a reasonably small number of manifolds. We must also establish that the examples we encounter are connected to each other by other

examples, with each example surrounded by other highly similar examples that may be reached by applying transformations to traverse the manifold. The second argument in favor of the manifold hypothesis is that we can also imagine such neighborhoods and transformations, at least informally. In the case of images, we can certainly think of many possible transformations that allow us to trace out a manifold in image space: we can gradually dim or brighten the lights, gradually move or rotate objects in the image, gradually alter the colors on the surfaces of objects, etc. It remains likely that there are multiple manifolds involved in most applications. For example, the manifold of images of human faces may not be connected to the manifold of images of cat faces.

These thought experiments supporting the manifold hypotheses convey some intuitive reasons supporting it. More rigorous experiments (Cayton, 2005; Narayanan and Mitter, 2010; Schölkopf *et al.*, 1998; Roweis and Saul, 2000; Tenenbaum *et al.*, 2000; Brand, 2003; Belkin and Niyogi, 2003; Donoho and Grimes, 2003; Weinberger and Saul, 2004) clearly support the hypothesis for a large class of datasets of interest in AI.

When the data lies on a low-dimensional manifold, it can be most natural for machine learning algorithms to represent the data in terms of coordinates on the manifold, rather than in terms of coordinates in $\mathbb{R}^n$. In everyday life, we can think of roads as 1-D manifolds embedded in 3-D space. We give directions to specific addresses in terms of address numbers along these 1-D roads, not in terms of coordinates in 3-D space. Extracting these manifold coordinates is challenging, but holds the promise to improve many machine learning algorithms. This general principle is applied in many contexts. Figure 5.13 shows the manifold structure of a dataset consisting of faces. By the end of this book, we will have developed the methods necessary to learn such a manifold structure. In figure 20.6, we will see how a machine learning algorithm can successfully accomplish this goal.

This concludes part I, which has provided the basic concepts in mathematics and machine learning which are employed throughout the remaining parts of the book. You are now prepared to embark upon your study of deep learning.