

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 $10\times10=100$ 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 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 x, we can just return the number of training examples in the same unit volume cell as 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