Introduction to Machine Learning

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Abstract

This is a lecture note for the course CSCI-UA.0473-001 (Intro to Machine Learning) at the Department of Computer Science, Courant Institute of Mathematical Sciences at New York University. The content of the lecture note was selected to fit a single 12-week-long course (3 hours a week) and to mainly serve undergraduate students majoring in computer science. Many existing materials in machine learning therefore had to be omitted.

For a more complete coverage of machine learning (with math!), the following text books are recommended in addition to this lecture note:

- "Pattern Recognition and Machine Learning" by Chris Bishop [1]
- "Machine Learning: a probabilistic perspective" by Kevin Murphy [3]
- "A Course in Machine Learning" by Hal Daumé[1]

For practical exercises, Python scripts based on numpy and scipy are available at `https://github.com/nyu-dl/Intro_to_ML_Lecture_Note/tree/master/notebook`. They are under heavy development and subject to frequent changes over the course. I recommend you to check back frequently. Again, these are not exhaustive, and for a more complete coverage on machine learning practice, I recommend the following book:

- "Introduction to Machine Learning with Python" by Andreas Müller and Sarah Guido

Note that those sections marked with $\star$ are optional and will not be covered during regular lectures. They will likely not be filled in by the end of the first round of the lectures either..

[1] Available at `http://ciml.info/`.

Notations

Throughout this lecture note, I will use the following notational conventions:

- A bold-faced lower-case alphabet is used for a vector: $\mathbf{x}$
- A bold-faced upper-case alphabet is used for a matrix: $\mathbf{W}$
- A lower-case alphabet is often used for a scalar: x, η
- A lower-case alphabet is also used for denoting a function
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Chapter 1

Classification

1.1 Supervised Learning

In supervised learning, our goal is to build or find a machine M that takes as input a multi-dimensional vector $\mathbf{x} \in \mathbb{R}^d$ and outputs a response vector $\mathbf{y} \in \mathbb{R}^{d'}$. That is,

$$M : \mathbb{R}^d \to \mathbb{R}^{d'}.$$

Of course this cannot be done out of blue, and we first assume that there exists a reference design M^* of such a machine. We then refine our goal as to build or find a machine M that imitates the reference machine M^* as closely as possible. In other words, we want to make sure that for any given $\mathbf{x}$, the outputs of M and M^* coincide, i.e.,

$$M(\mathbf{x}) = M^*(\mathbf{x}), \text{ for all } \mathbf{x} \in \mathbb{R}^d. \tag{1.1}$$

This is still not enough for us to find M, because there are infinitely many possible M's through which we must search. We must hence decide on our *hypothesis set* H of potential machines. This is an important decision, as it directly influences the difficulty in finding such a machine. When your hypothesis set is not constructed well, there may not be a machine that satisfies the criterion above.

We can state the same thing in a slightly different way. First, let us assume a function D that takes as input the output of M^*, a machine M and an input vector $\mathbf{x}$, and returns how much they differ from each other, i.e.,

$$D : \mathbb{R}^{d'} \times H \times \mathbb{R}^{d'} \to \mathbb{R}_+,$$

where $\mathbb{R}_+$ is a set of non-negative real numbers. As usual in our everyday life, the smaller the output of D the more similar the outputs of M and M^*. An example of such a function would be

$$D(y, M, \mathbf{x}) = \begin{cases} 0, & \text{if } y = M(\mathbf{x}) \\ 1, & \text{otherwise} \end{cases}.$$

It is certainly possible to tailor this distance function, or a *per-example cost* function, for a specific target task. For instance, consider an intrusion detection system M which takes as input a video frame of a store front and returns a binary indicator, instead of a real number, whether there is a thief in front of the store (0: no and 1: yes). When there is no thief ($M^*(\mathbf{x}) = 0$), it does not cost you anything when M agrees with M^*, but you must pay \$10 for security dispatch if M predicted 1. When there is a thief in front of your store ($M^*(\mathbf{x}) = 1$), you will lose \$100 if the alarm fails to detect the thief ($M(\mathbf{x}) = 0$) but will not lose any if the alarm went off. In this case, we may define the per-example cost function as

$$D(y, M, \mathbf{x}) = \begin{cases} 0, & \text{if } y = M(\mathbf{x}) \\ -10, & \text{if } y = 0 \text{ and } M(\mathbf{x}) = 1 \\ -100, & \text{if } y = 1 \text{ and } M(\mathbf{x}) = 0 \end{cases}.$$

Note that this distance is asymmetric.

Given a distance function D, we can now state the supervised learning problem as finding a machine M, with in a given hypothesis set H, that minimizes its distance from the reference machine M^* for any given input. That is,

$$\arg\min_{M \in H} \int_{\mathbb{R}^d} D(M^*(\mathbf{x}), M, \mathbf{x}) \mathrm{d}\mathbf{x}. \tag{1.2}$$

You may have noticed that these two conditions in Eqs. (1.1)–(1.2) are not equivalent. If a machine M satisfies the first condition, the second conditions is naturally satisfied. The other way around however does not necessarily hold. Even then, we prefer the second condition as our ultimate goal to satisfy in machine learning. This is because we often cannot guarantee that M^* is included in the hypothesis set H. The first condition simple becomes impossible to satisfy when $M^* \notin H$, but the second condition gets us a machine M that is *close* enough to the reference machine M^*. We prefer to have a suboptimal solution rather than having no solution.

The formulation in Eq. (1.2) is however not satisfactory. Why? Because not every point $\mathbf{x}$ in the input space $\mathbb{R}^d$ is born equal. Let us consider the previous example of a video-based intrusion detection system again. Because the camera will be installed in a fixed location pointing toward the store front, video frames will generally look similar to each other, and will only form a very small subset of all possible video frames, unless some exotic event happens. In this case, we would only care whether our alarm M works well for those frames showing the store front and people entering or leaving the store. Whether the distance between the reference machine and my alarm is small for a video frame showing the earth from the outer space would not matter at all.

And, here comes probability. We will denote by $p_X(\mathbf{x})$ the probability (density) assigned to the input $\mathbf{x}$ under the distribution X, and assume that this probability reflects how likely the input $\mathbf{x}$ is. We want to emphasize the impact of the distance D on likely inputs (high $p_X(\mathbf{x})$) while ignoring the impact on unlikely inputs (low $p_X(\mathbf{x})$). In other words, we weight each per-example cost with the probability of the corresponding example. Then the problem of supervised learning becomes

$$\arg\min_{M \in H} \int_{\mathbb{R}^d} p_X(\mathbf{x}) D(M^*(\mathbf{x}), M, \mathbf{x}) \mathrm{d}\mathbf{x} = \arg\min_{M \in H} \mathbb{E}_{\mathbf{x} \sim X} \left[D(M^*(\mathbf{x}), M, \mathbf{x}) \right]. \tag{1.3}$$

Are we done yet? No, we still need to consider one more hidden cost in order to make the description of supervised learning more complete. This hidden cost comes from the operational cost, or *complexity*, of each machine M in the hypothesis set H. It is reasonable to think that some machines are cheaper or more desirable to use than some others are. Let us denote this cost of a machine by $C(M)$, where $C : H \to \mathbb{R}_+$. Our goal is now slightly more complicated in that we want to find a machine that minimizes both the cost in Eq. (1.3) and its operational cost. So, at the end, we get

$$\arg\min_{M \in H} \underbrace{\mathbb{E}_{\mathbf{x} \sim X} \left[D(M^*(\mathbf{x}), M, \mathbf{x}) \right] + \lambda C(M)}_{R=\text{Expected Cost}}, \tag{1.4}$$

where $\lambda \in \mathbb{R}_+$ is a coefficient that trades off the importance between the expected distance (between M^* and M) and the operational cost of M.

In summary, supervised learning is a problem of finding a machine M such that has bot the low expectation of the distance between the outputs of M^* and M over the input distribution and the low operational cost.

In Reality It is unfortunately impossible to solve the minimization problem in Eq. (1.4) in reality. There are so many reasons behind this, but the most important reason is the input distribution p_X or lack thereof. We can decide on a distance function D ourselves based on our goal. We can decide ourselves a hypothesis set H ourselves based on our requirements and constraints. All good, but p_X is not controllable in general, as it reflects how the world is, and the world does not care about our own requirements nor constraints.

Let's take the previous example of video-based intrusion system. Our reference machine M^* is a security expert who looks at a video frame (and a person within it) and determines whether that person is an intruder. We may decide to search over any arbitrary set of neural networks to minimize the expected loss. We have however absolutely no idea what the precise probability $p(\mathbf{x})$ of any video frame. Instead, we only observe $\mathbf{x}$'s which was randomly sampled from the input distribution by the surrounding environment. We have no access to the input distribution itself, but what comes out of it.

We only get to observe a *finite* number of such samples $\mathbf{x}$'s, with which we must approximate the expected cost in Eq. (1.4). This approximation method, that is approximation based on a finite set of samples from a probability distribution, is called a *Monte Carlo method*. Let us assume that we have observed N such samples: $\left\{\mathbf{x}^1, \ldots, \mathbf{x}^N\right\}$. Then we can approximate the expected cost by

$$\underbrace{\mathbb{E}_{\mathbf{x} \sim X} \left[D(M^*(\mathbf{x}), M, \mathbf{x}) \right] + \lambda C(M)}_{\text{Expected Cost}} = \underbrace{\frac{1}{N} \sum_{n=1}^{N} D(M^*(\mathbf{x}^n), M, \mathbf{x}^n) + \lambda C(M)}_{\tilde{R}=\text{Empirical Cost}} + \varepsilon, \tag{1.5}$$

where ε is an approximation error. We will call this cost, computed using a finite set of input vectors, an *empirical cost*.

Inference We have so far talked about what is a correct way to find a machine M for our purpose. We concluded that we want to find M by minimizing the empirical cost in Eq. (1.5). This is a good start, but let's discuss why we want to do this first. There may be many reasons, but often a major complication is the expense of running the reference machine M^* or the limited access to the reference machine M^*. Let us hence make it more realistic by assuming that we will have access to M^* only once at the very beginning together with a set of input examples. In other words, we are given

$$D_{\text{tra}} = \left\{ (\mathbf{x}^1, M^*(\mathbf{x}^1)), \ldots, (\mathbf{x}^N, M^*(\mathbf{x}^N)) \right\},$$

to which we refer as a *training set*. Once this set is available, we can find M that minimizes the empirical cost from Eq. (1.5) without ever having to query the reference machine M^*.

Now let us think of what we would do when there is a *new* input $\mathbf{x} \notin D_{\text{tra}}$. The most obvious thing is to use $\hat{M}$ that minimizes the empirical cost, i.e., $\hat{M}(\mathbf{x})$. Is there any other way? Another way is to use all the models in the hypothesis set, instead of using only one model. Obviously, not all models were born equal, and we cannot give all of them the same chance in making a decision. Preferably we give a higher weight to the machine that has a lower empirical cost, and also we want the weights to sum to 1 so that they reflect a properly normalized proportion. Thus, let us (arbitrarily) define, as an example, the weight of each model as:

$$\omega(M) = \frac{1}{Z} \exp\left(-J(M, D_{\text{tra}})\right),$$

where J corresponds to the empirical cost, and

$$Z = \sum_{M \in H} \exp\left(-J(M, D_{\text{tra}})\right)$$

is a normalization constant.

With all the models and their corresponding weights, I can now think of many strategies to *infer* what the output of M^* given the new input $\mathbf{x}$. Indeed, the first approach we just talked about corresponds to simply taking the output of the model that has the highest weight. Perhaps, I can take the weighted average of the outputs of all the machines:

$$\sum_{M \in H} \omega(M) M(\mathbf{x}), \tag{1.6}$$

which is equivalent to $\mathbb{E}\left[M(\mathbf{x})\right]$ under our arbitrary construction of the weights.[1] We can similarly check the variance of the prediction. Perhaps I want to inspect a set of outputs from the top-K machines according to the weights.

We will mainly focus on the former approach, which is often called *maximum a posteriori* (MAP), in this course. However, in a few of the lectures, we will also consider the latter approach in the framework of *Bayesian* modelling.

[1] *Is it really arbitrary, though?*

1.2 Perceptron

Let us examine how this concept of supervised learning is used in practice by considering a binary classification task. Binary classification is a task in which an input vector $\mathbf{x} \in \mathbb{R}^d$ is classified into one of two classes, negative (0) and positive (1). In other words, a machine M takes as input a d-dimensional vector and outputs one of two values.

Hypothesis Set In perceptron, a hypothesis set is defined as

$$H = \left\{ M | M(\mathbf{x}) = \text{sign}(\mathbf{w}^\top \tilde{\mathbf{x}}), \mathbf{w} \in \mathbb{R}^{d+1} \right\},$$

where $\tilde{\mathbf{x}} = [\mathbf{x}; 1]$ denotes concatenating 1 at the end of the input vector $\mathbf{x}$,[2] and

$$\text{sign}(x) = \begin{cases} 0, & \text{if } x \leq 0, \\ 1, & \text{otherwise} \end{cases} . \tag{1.7}$$

In this section, we simply assume that each and every machine in this hypothesis set has a constant operational cost c, i.e., $C(M) = c$ for all $M \in H$.

Distance rewrite!

Given an input $\mathbf{x}$, we now define a distance between M^* and M. In particular, we will use the following distance function:[3]

$$D(M^*(\mathbf{x}), M, \mathbf{x}) = -\underbrace{(M^*(\mathbf{x}) - M(\mathbf{x}))}_{\text{(a)}} \underbrace{\left(\mathbf{w}^\top \tilde{\mathbf{x}}\right)}_{\text{(b)}}. \tag{1.8}$$

The term (a) states that the distance between the predictions of the reference and our machines is 0 as long as their predictions coincide. When it is not, the term (a) will be 1 if $M^*(\mathbf{x}) = 1$ and -1 if $M^*(\mathbf{x}) = 0$.

When it is not, the term (a) will be 1, which is when the term (b) comes into play. The dot product in (b) computes how well the weight vector $\mathbf{w}$ and the input vector $\mathbf{x}$ aligns with each other.[4] When they are positively aligned (pointing in the same direction), this term will be positive, making the output of the machine 1. When they are negative aligned (pointing in opposite directions), it will be negative with the output of the machine M 0.

Considering both (a) and (b), we see that the smallest value D can take is 0 ,when the prediction is correct,[5] and otherwise, positive. When the term (a) is 1, $\mathbf{w}^\top \tilde{\mathbf{x}}$ is negative, because $M(\mathbf{x})$ was 0, and the overall distance becomes positive (note the

[2] Why do we augment the original input vector $\mathbf{x}$ with an extra 1? What is an example in which this extra 1 is necessary? This is left to you as a **homework assignment**.

[3] There is a problem with this distance function. What is it? This is left to you as a **homework assignment**.

[4] $\mathbf{w}^\top \tilde{\mathbf{x}} = \sum_{i=1}^{d+1} w_i x_i$.

[5] There is one more case. What is it?

negative sign at the front.) When the term (b) is -1, $\mathbf{w}^\top \tilde{\mathbf{x}}$ is positive, because $M(\mathbf{x})$ was 1, in which case the distance is again positive.

What should we do in order to decrease this distance, if it is non-zero? We want to make the weight vector $\mathbf{w}$ to be aligned more positively with $M^*(\mathbf{x})$, if the term (a) is 1, which can be done by moving $\mathbf{w}$ toward $\tilde{\mathbf{x}}$. In other words, the distance D shrinks if we add a bit of $\tilde{\mathbf{x}}$ to $\mathbf{w}$, i.e., $\mathbf{w} \leftarrow \mathbf{w} + \eta \tilde{\mathbf{w}}$. If the term (a) is -1, we should instead push $\mathbf{w}$ so that it will *negatively* align with $\tilde{\mathbf{x}}$, i.e., $\mathbf{w} \leftarrow \mathbf{w} - \eta \tilde{\mathbf{w}}$. These two cases can be unified by

$$\mathbf{w} \leftarrow \mathbf{w} + \eta \left(M^*(\mathbf{x}) - M(\mathbf{x})\right) \tilde{\mathbf{x}}, \tag{1.9}$$

where η is often called a *step size* or *learning rate*. We can repeat this update until the term (a) in Eq. (1.8) becomes 0.

Learning As discussed earlier, we assume that we make only a finite number of queries to the reference machine M^* using a set of inputs drawn from the unknown input distribution $p(\mathbf{x})$. This results in our training dataset:

$$D_{\text{tra}} = \left\{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_N, y_N)\right\},$$

where we begin to use a short hand $y_n = M^*(\mathbf{x}_n)$.

With this dataset, our goal now is to find $M \in H$ that has the least empirical cost in Eq. (1.5) with the distance function defined in Eq. (1.8). Combining these two, we get

$$J(\mathbf{w}, D_{\text{tra}}) = -\frac{1}{N} \sum_{n=1}^{N} \left(y_n - M(\mathbf{x}_n)\right) \left(\mathbf{w}^\top \tilde{\mathbf{x}_n}\right). \tag{1.10}$$

We will again resort to an iterative method for minimizing this empirical cost function, as we have done with a single input vector above. What we will do is to collect all those input vectors on which M (or equivalently $\mathbf{w}$) has made mistakes. This is equivalent to considering only those input vectors where $y_n - M(\mathbf{x}_n) \neq 0$. Then, we collect all the *update directions*, computed using Eq. (1.9), and move the weight vector $\mathbf{w}$ toward its average. That is,

$$\mathbf{w} \leftarrow \mathbf{w} + \eta \frac{1}{N} \sum_{n=1}^{N} \left(y_n - M(\mathbf{x}_n)\right) \tilde{\mathbf{x}}. \tag{1.11}$$

We apply this rule repeatedly until the empirical cost in Eq. (1.10) does not improve (i.e., decrease).

This learning rule is known as a *perceptron learning rule*, which was proposed by Rosenblatt in 1950's [4], and has a nice property that it will find a correct M in the sense that the empirical cost is at its minimum (0), *if* such M is in H. In other words, if our hypothesis set H is good and includes a reference machine M^*, this perceptron learning rule will eventually find an equally good machine M. It is important to note that there may be many such M, and the perceptron learning rule will find one of them.

1.3 Logistic Regression

The perceptron is not entirely satisfactory for a number of reasons. One of them is that it does not provide a well-calibrated measure of the degree to which a given input is either negative or positive. That is, we want to know not whether it is negative or positive but rather how likely it is negative. It is then natural to build a machine that will output the probability $p(C|\mathbf{x})$, where $C \in \{-1, 1\}$.

Hypothesis Set To do so, let us first modify the definition of a machine M. M now takes as input a vector $\mathbf{x} \in \mathbb{R}^d$ and returns a probability $p(C|\mathbf{x}) \in [0, 1]$ rather than $\{0, 1\}$. We only need to change just one thing from the perceptron, that is

$$M(\mathbf{x}) = \sigma(\mathbf{w}^\top \tilde{\mathbf{x}}), \tag{1.12}$$

where σ is a sigmoid function defined as

$$\sigma(a) = \frac{1}{1 + \exp(-a)}$$

and is bounded by 0 from below and by 1 from above. Suddenly this machine does not return the prediction, but the probability of the prediction being positive (1). That is,

$$p(C = 1|\mathbf{x}) = M(\mathbf{x}).$$

Naturally, our hypothesis set is now

$$H = \left\{ M | M(\mathbf{x}) = \sigma(\mathbf{w}^\top \tilde{\mathbf{x}}), \mathbf{w} \in \mathbb{R}^{d+1} \right\},$$

where $\tilde{\mathbf{x}} = [\mathbf{x}; 1]$ denotes concatenating 1 at the end of the input vector as before.

Distance The distance is not trivial to define in this case, because the things we want to measure the distance between are not directly comparable. One is an element in a discrete set (0 or 1), and the other is a probability. It is helpful now to think instead about *how often* a machine M will agree with the reference machine M^*, if we randomly sample the prediction given its output distribution $p(C|\mathbf{x})$. This is exactly equivalent to $p(C = M^*(\mathbf{x})|\mathbf{x})$. In this sense, the distance between the reference machine M^* and our machine M given an input vector $\mathbf{x}$ is smaller than this frequency of M being correct is larger, and vice versa. Therefore, we define the distance as the negative log-probability of the M's output being correct:

$$\begin{aligned} D(M^*(\mathbf{x}), M, \mathbf{x}) &= -\log p(C = M^*(\mathbf{x})|\mathbf{x}) \\ &= -\left(M^*(\mathbf{x}) \log M(\mathbf{x}) + (1 - M^*(\mathbf{x})) \log(1 - M(\mathbf{x}))\right), \end{aligned} \tag{1.13}$$

where $p(C = 1|\mathbf{x}) = M(\mathbf{x})$. The latter equality comes from the definition of *Bernoulli distribution*.[6]

[6] give a brief def of Bernoulli distribution

With this definition of our distance, how do we adjust $\mathbf{w}$ of M to lower it? In the case of perceptron, we were able to manually come up with an *algorithm* by looking at the perceptron distance in Eq. (1.8). It is however not too trivial with this logistic regression distance.[7] Thus, we now turn to Calculus, and use the fact that the *gradient* of a function points to the direction toward which its output increases (at least locally).

The gradient of the above logistic regression distance function with respect to the weight vector $\mathbf{w}$ is[8]

$$\nabla_{\mathbf{w}} D(M^*(\mathbf{x}), M, \mathbf{x}) = -(M^*(\mathbf{x}) - M(\mathbf{x}))\tilde{\mathbf{x}}. \tag{1.14}$$

When we move the weight vector ever so slightly in the opposite direction, the logistic regression distance in Eq. (1.13) will decrease. That is,

$$\mathbf{w} \leftarrow \mathbf{w} + \eta\,(M^*(\mathbf{x}) - M(\mathbf{x}))\,\tilde{\mathbf{x}}, \tag{1.15}$$

where $\eta \in \mathbb{R}$ is a small scalar and called either a *step size* or *learning rate*.

Coincidence? Is it surprising to realize that this rule for logistic regression is identical to the perceptron rule in Eq. (1.9)? Let us see what this logistic regression rule, or equivalent to perceptron learning rule, does by focusing on the update term (the second term in the learning rule). The first multiplicative factor $(M^*(\mathbf{x}) - M(\mathbf{x}))$ can be written as

$$M^*(\mathbf{x}) - M(\mathbf{x}) = \underbrace{\overline{\text{sign}}(M^*(\mathbf{x}) - M(\mathbf{x}))}_{\text{(a)}} \underbrace{|M^*(\mathbf{x}) - M(\mathbf{x})|}_{\text{(b)}}, \tag{1.16}$$

where

$$\overline{\text{sign}}(x) = \begin{cases} -1, & \text{if } x \leq 0, \\ 1, & \text{otherwise} \end{cases}$$

is a symmetric sign function (compare it to the asymmetric sign function in Eq. (1.7).)

The term (a) effectively tell us *in which way* the machine is wrong about the input $\mathbf{x}$. Is M saying it is likely to be 0 when the reference machine says 1, or is M saying it is likely to be 1 when the reference machine says 0? In the former case, we want the weight vector $\mathbf{w}$ to align more with $\mathbf{x}$, and thus the positive sign. In the latter case, we want the opposite, and hence the negative sign. The second term (b) tells us *how much* the machine is wrong about the input $\mathbf{x}$. This term ignores in which direction the machine is wrong, since it is computed by the term (a), but entirely focuses on how *far* the model's prediction is from that of the reference machine. If the prediction is close to that of the reference machine, we only want the weight vector to move ever so slowly.

The second term in both the logistic regression and perceptron rules is the input vector, augmented with an extra 1. This term is there, because the prediction by a machine M is made based on how well the weight vector and the input vector align with each other, which is computed as a dot product between these two vectors.

[7] It may be trivial to some who have great mathematical intuition.

[8] The step-by-step derivation of this is left to you as a **homework assignment**.

In other words, it is not a coincidence, but only natural that they are equivalent, as both of them effectively solve the same problem of binary classification. In the case of perceptron, we have reached its learning rule based on our observation of the process, while in the case of logistic regression, we relied on a more mechanical process of using gradient to find the steepest ascent direction. The latter approach is often more desirable, as it allows us to apply the same procedure (update the machine following the steepest descent direction,) however with a constraint that the empirical cost be differentiable (almost everywhere[9]) with respect to the machine's parameters. We will thus largely stick to this kind of gradient-based optimization to minimize any distance function from here on.

The only major difference between the learning rules for the logistic regression and perceptron is whether the term (b) in Eq. (1.16) is discrete (in the case of perceptron) or continuous (in the case of logistic regression.) More specifically, the term (b) in the perceptron learning rule is either 0 or 1.

Learning With the distance function defined, we can write a full empirical cost as

$$J(\mathbf{w}, D_{\text{tra}}) = -\frac{1}{N}\sum_{n=1}^{N} y_n \log M(\mathbf{x}_n) + (1-y_n)\log(1-M(\mathbf{x}_n)).$$

We assume that the operational cost, or complexity, of each M can be ignored. Similarly to what we have done for minimizing (decreasing) the distance between M and M^* given a single input vector, we will use the gradient of the whole empirical cost function to decide how we change the weight vector $\mathbf{w}$. The gradient is

$$\nabla_{\mathbf{w}} J = -\frac{1}{N}\sum_{n=1}^{N} \nabla_{\mathbf{w}} D(y_n, M, \mathbf{x}_n),$$

which is simply the average of the gradients of the distances from Eq. (1.14) over the whole training set.

The fact that the empirical cost function is (twice) differentiable with respect to the weight vector allows us to use any advanced gradient-based optimization algorithm. Perhaps even more importantly, we can use automatic differentiation to compute the gradient of the empirical cost function *automatically*.[10]

[9] We will see why the cost function does not have to be differentiable everywhere later in the course.

[10] Some of widely-used software packages that implement automatic differentiation include

- Autograd for Python: `https://github.com/HIPS/autograd`
- Autograd for Torch: `https://github.com/twitter/torch-autograd`
- Theano: `http://deeplearning.net/software/theano/`
- TensorFlow: `https://www.tensorflow.org/`

Throughout this course, we will use Autograd for Python for demonstration.

1.4 Overfitting, Regularization and Complexity

1.4.1 Overfitting: Generalization Error

At the very beginning of this course, we have talked about two cost functions; (1) expected cost in Eq. (1.4) and (2) empirical cost in Eq. (1.5).[11] We loosely stated that we find a machine that minimizes the empirical cost $\tilde{R}$ because we cannot compute the expected cost R, somehow hoping that the approximation error ε (from Eq. (1.5)) would be small. Let's discuss this a bit more in detail here.

Let us define the generalization error as a difference between the empirical and expected cost functions given a reference machine M^*, a machine M and a training set D_{tra}:

$$G(M^*, M, D_{\text{tra}}) = R(M^*, M) - \tilde{R}(M^*, M, D_{\text{tra}}). \tag{1.17}$$

We can further define its expectation as

$$\bar{G}(M^*, M) = R(M^*, M) - \mathbb{E}_{D\sim P}\left[\tilde{R}(M^*, M, D)\right], \tag{1.18}$$

where P is the data distribution.

When this generalization error is large, it means that we are hugely overestimating how good the machine M is compared to the reference machine M^*. Although M is not really good, i.e., the expected cost R is high, M is good on the training set D_{tra}, i.e., the empirical cost $\tilde{R}$ is low. This is precisely the situation we want to avoid: we do not want to brag our machine is good when it is in fact a horrible approximation to the reference machine M^*. In this embarrassing situation, we say that the machine M is *overfitting* to the training data.

Unlike how I said earlier, the goal of supervised learning, or machine learning in general, is therefore to search for a machine in a hypothesis set not only to minimize the empirical cost function but also to minimize the generalization error. In other words, we want to find a machine that simultaneously minimizes the empirical cost function and avoids overfitting.

Statistical learning theory, a major subfield of machine learning, largely focuses on computing the upper-bound of the generalization error. The bound, which is often probabilistic, is often a function of, for instance, the dimensionality of an input vector $\mathbf{x}$ and a hypothesis set. This allows us to understand how well we should expect our learning setting to work, in terms of generalization error, even *without* testing it on actual data. Awesome, but we will skip this in this course, as the upper-bound is often too loose, and rough sample-based approximation of the generalization error works better in practice.[12]

1.4.2 Validation

In practice, the generalization error itself is rarely of interest. It is rather the expected cost function R of a machine M that interests us, because we will eventually pick one

[11] Note that the complexity, or operational cost, of a machine M is often *not* included in either of the cost functions, but this is not a problem to include them as long as both cost functions have them.

[12] *Well, the better answer is that it involves too much math..*

M that has the least expected cost.[13] But, again, we cannot really compute the expected cost function and must resort to an approximate method. As done for training, we again use a set D_{val} of samples from the data distribution to estimate the expected cost, as in Eq. (1.5), that is[14]

$$\tilde{R}_{\text{val}} = \frac{1}{N'} \sum_{(y,\mathbf{x}) \in D_{\text{val}}} D(y, M, \mathbf{x}) + \lambda C(M).$$

In order to avoid any bias in estimating the expected cost function, via this validation cost, we must use a validation set D_{val} *independent* from the training set D_{tra}. We ensure this in practice by splitting a given training set into two disjoint subsets, or partitions, and use them as training and validation sets.

This is how we will estimate the expected cost of a trained model M. How are we going to use it? Let us consider having more than one hypothesis set H_l for $m = l, \ldots, L$. Given a training set D_{tra} and one of hypothesis sets H_l, we will find a machine $M^l \in H_l$ that minimizes the empirical cost function:

$$M^l = \operatorname*{arg\,min}_{M \in H_l} \tilde{R}(M, D_{\text{tra}}).$$

We now have a set of trained models $\left\{M^1, \ldots, M^L\right\}$, and we must choose one of them as our final solution. In doing so, we use the validation cost computed using a *separate* validation set D_{val} which approximates the expected cost. We choose the one with the smallest validation cost among the L trained models:

$$\hat{M} = \operatorname*{arg\,min}_{M^l | l=1,\ldots,L} \tilde{R}_{\text{val}}(M^l, D_{\text{val}}).$$

Example 1: Model Selection Let's take a simple example of having two hypothesis sets. One hypothesis set $H_{\text{perceptron}}$ contains all possible perceptrons, and the other set H_{logreg} has all possible logistic regressions. We will find one perceptron and one logistic regression from these hypothesis sets by using the learning rules we learned earlier (Eq. (1.11) and Eq. (1.15)). We select one of these two *models* based not on the empirical cost function but on the validation cost function.

Example 2: Early Stopping Can this be useful even if we have a single hypothesis set? Indeed. So far, two families of classifiers we have considered, which are perceptrons and logistic regression, learning happened iteratively. That is, we slowly evolve the parameters, or more specifically the weight vector. Let us denote the weight vector after the l-th update by $\mathbf{w}^l$, and assume that we have applied the learning rule L-many times. Suddenly I have L different classifiers, just like what we had with L different classifiers earlier when there were L hypothesis sets.[15] Instead of taking the very last

[13] Though, as we discussed earlier in Eq. (1.6), it may be better to keep more than one M in certain cases.

[14] It is a usual practice to omit the model complexity term when computing the validation cost. We will get to why this is so shortly.

[15] In some sense, we can view each of these classifiers as coming from L different (overlapping) hypothesis sets. Each hypothesis set can be characterized as *reachable* in l gradient updates from the initial weight vector.

weight vector $\mathbf{w}^L$, we will choose

$$\hat{M} = \underset{M^l | l=1,\ldots,L}{\arg\min}\ \tilde{R}_{\text{val}}(M^l, D_{\text{val}}),$$

where M^l is a classifier with its weight vector $\mathbf{w}^l$. This technique is often referred to as *early stopping*, and is a crucial recipe in iterative learning.

Cross-Validation Often we are not given a large enough set of examples to afford dividing it into two sets, and using only one of them to train competing models. Either the training set would be too small for the empirical (training) cost to well approximate the expected cost, or the validation set would be too small for the validation cost to be meaningful when selecting the final model (or the correct hypothesis set.) In this case, we use a technique called *K-fold cross validation*.

We first evenly split a given training set D_{tra} into K partitions while ensuring that the statistics of all the partitions are roughly similar, for instance, by ensuring that the label proportion (the number of positive examples to that of the negative examples) stays same. For each hypothesis set H, we train K classifiers, where D_{tra}
D^k_{tra} is used to train the k-th classifier and D^k_{tra} to compute its validation cost. We then get K validation costs of which the average is our estimate of the empirical cost of the current hypothesis set. We essentially reuse each example $K-1$ times for training and $K-1$ times for validation, thereby increasing both the efficiency of our use of training examples as well as the stability of our estimate. When K is set to the number of all training examples, we call it leave-one-out cross-validation (LOOCV).

Cross-validation is a good approach for model selection, but not usable for early-stopping.[16] Furthermore, when the training set is large, it may easily become infeasible to try cross-validation, as the computational complexity grows linearly with respect to K. It is however a recommended practice to use cross-validation whenever you have a manageable size of training examples.

Test Set As soon as we use the validation set to *select* among multiple hypothesis sets or models, the validation cost of the final model is not anymore a good estimate of its expected cost. This is largely because again of overfitting. Our choice of hypothesis set or model will agree well with the validation cost, but unavoidably the validation cost will have its own generalization error. Thus, we need yet another set of examples based on which we estimate the true expected cost. This set of examples is often called a *test set*.

Most importantly, *the test set must be withheld* throughout the whole process of learning *until the very end*. As soon as any intermediate decision about learning, such as the choice of hypothesis set, is made based on the test set, your estimate of the expected cost of the final model becomes biased. Thus, in practice, what you must do is to split a training set into three portions; training, validation and test partitions, in advance of anything you do. Is there an ideal split? No.

Similarly to how we estimated the validation cost, it is often the case in which you do not have enough data and cannot afford to withhold a substantial portion of it

[16] **Homework assignment**: Why is cross-validation not a feasible strategy for early-stopping?

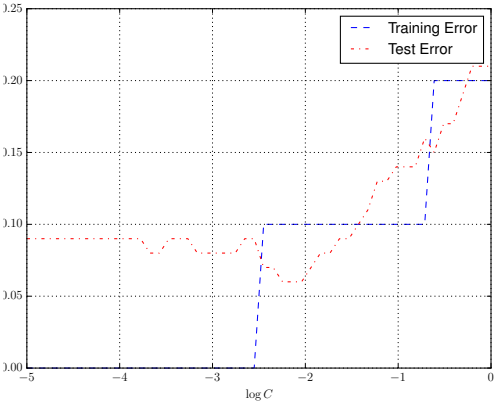


Figure 1.1: Training and test errors with respect to the weight decay coefficient. Notice that the test error grows back even when the training error is 0 as the weight decay coefficient decreases.

as a test set. In that case, it is also a good practice to employ the strategy of K-fold cross-validation. In this case, it is worth noting that you need *nested* K-fold cross-validation. That is, for each k-th fold from the outer cross-validation loop, you use the inner cross-validation (K iterations of training and validation) for model selection. It is computationally expensive, as now it grows quadratically with respect to K, i.e., $O(K^2)$, but this is the best practice to accurately estimate the expected cost of your learning algorithm given only a small number of training examples.

1.4.3 Overfitting and Regularization

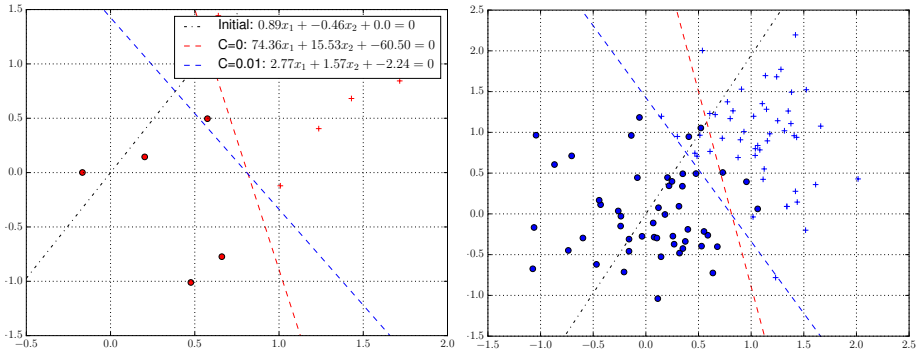
We now know how to measure the degree of overfitting by approximately computing the difference between the expected cost and the empirical cost. In this section, let us think of how we can use this in more detail. Let us start from the "Example 1: Model Selection" from above.

When we select a model, the first question that needs to be answered is what are our hypothesis sets.

1.5 One Classifier, Many Loss Functions

1.5.1 Classification as Scoring

Let us use f as a shorthand for denoting the dot product between the weight vector $\mathbf{w}$ and an input vector $\mathbf{x}$ augmented with an extra 1, that is $f(\mathbf{x};\mathbf{w}) = \mathbf{w}^\top \tilde{\mathbf{x}}$. Instead of $y \in \{0,1\}$ as a set of labels (negative and positive), we will switch to $y \in \{-1,1\}$ to



(a) Training Set (b) Test Set

Figure 1.2: Both solutions of logistic regression perfectly fit the training set regardless of whether weight decay regularization was used. However, it is clear that the model with the optimal weight decay coefficient (blue line) classifies the test set better.

make later equations less cluttered. Now, let us define a score function[17] that takes as input an input vector $\mathbf{x}$, the correct label y (returned by a reference machine M^*) and the weight vector (or you can say the machine M itself):

$$s(y, \mathbf{x}; M) = y\mathbf{w}^\top \tilde{\mathbf{x}}. \tag{1.19}$$

Given any machine that performs binary classification, such as perceptron and logistic regression, this score function tells us whether a given input vector $\mathbf{x}$ is correctly classified. If the score is larger than 0, it was correctly classified. Otherwise, the score would be smaller than 0. In other words, the score function defines a *decision boundary* of the machine M, which is defined as a set of points at which the score is 0, i.e.,

$$B(M) = \{\mathbf{x} | s(M(\mathbf{x}), \mathbf{x}; M) = 0\}.$$

When the score function s is defined as a linear function of the input vector $\mathbf{x}$ as in Eq. (1.19), the decision boundary corresponds to a linear hyperplane. In such a case, we call the machine a *linear classifier*, and if the reference machine M^* is a linear classifier, we call this problem of classification *linear separable*.

With this definition of a score function s, the problem of classification is equivalent to finding the weight vector $\mathbf{w}$, or the machine M, that positively scores each pair of an input vector and the corresponding label. In other words, our empirical cost function for classification is now

$$J(M, D_{\text{tra}}) = \frac{1}{|D_{\text{tra}}|} \sum_{(y,\mathbf{x}) \in D_{\text{tra}}} \underbrace{\overline{\text{sign}}(-s(y, \mathbf{x}; M))}_{D_{\text{0-1}}=\text{0-1 Loss}}. \tag{1.20}$$

[17] Note that the term "score" has a number of different meanings. For instance, in statistics, the score is defined as a gradient of the TODO

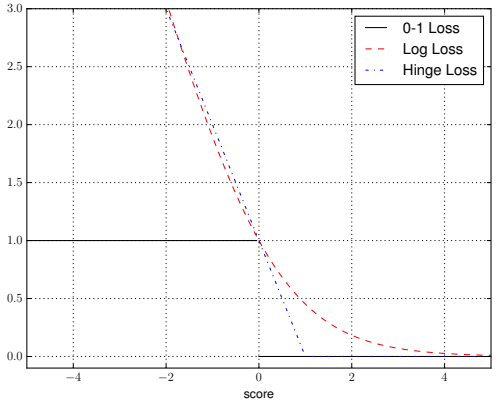


Figure 1.3: The figure plots three major loss functions–0-1 loss, log loss and hinge loss– with respect to the output of a score function s. Note that the log loss and hinge loss are upper-bound to the 0-1 loss.

Log Loss: Logistic Regression The distance[18] function of logistic regression in Eq. (1.13) can be re-written as

$$D_{\log}(y,\mathbf{x};M) = \frac{1}{\log 2}\log(1+\exp(-s(y,\mathbf{x};M))), \tag{1.21}$$

where $y \in \{-1,1\}$ instead of $\{0,1\}$, and the score function s is defined in Eq. (1.19).[19] This loss function is usually referred to as *log loss*.

How is this log loss related to the 0-1 loss from Eq. (1.20)? As shown in Fig. 1.3, the log loss is an upper-bound of the 0-1 loss. That is,

$$D_{\log}(y,\mathbf{x};M) \geq D_{0\text{-}1}(y,\mathbf{x};M) \text{ for all } s(y,\mathbf{x};M) \in \mathbb{R}.$$

1.5.2 Support Vector Machines: Max-Margin Classifier

Hinge Loss One potential issue with the log loss in Eq. (1.21) is that it is never 0:

$$D_{\log}(y,\mathbf{x};M) > 0.$$

Why is this an issue? Because it means that the machine M *wastes* its modelling capacity on pushing those examples as far away from the decision boundary as possible even if they were already correctly classified. This is unlike the 0–1 loss which ignores any correctly classified example.

Let us introduce another loss function, called *hinge loss*, which is defined as

$$D_{\text{hinge}}(y,\mathbf{x};M) = \max(0, 1 - s(y,\mathbf{x};M)).$$

[18] From here on, I will use both *distance* and *loss* to mean the same thing. This is done to make terminologies a bit more in line with how others use.

[19] **Homework assignment**: show that Eq. (1.13) and Eq. (1.21) are equivalent up to a constant multiplication for binary logistic regression.

Similarly to the log loss, the hinge loss is always greater than or equal to the zero-one loss, as can be seen from Fig. 1.3. We minimize this hinge loss and consequently minimize the 0–1 loss.[20]

What does this imply? It implies that minimizing the empirical cost function that is the sum of hinge losses will find a solution in which all the examples are at least a unit-distance (1) away from the decision boundary ($s(y,\mathbf{x};M)=0$). Once any example is further than a unit-distance away from *and* on the correct side of the decision boundary, there will not be any penalty, i.e., zero loss. This is contrary to the log loss which penalizes even correctly classified examples unless they are infinitely far away from and on the correct side of the boundary.

Max-Margin Classifier It is time for a thought experiment. We have only two unique training examples; one positive example $\tilde{\mathbf{x}}^+$ and one negative example $\tilde{\mathbf{x}}^-$. We can draw a line l between these two points. Any linear classifier perfectly classifies these two examples into their correct classes as long as the decision boundary, or *separating hyperplane*, meets the line l connecting the two examples. Because we are in the real space, there are infinitely many such classifiers. Among these infinitely many classifiers, which one should we use? Should the intersection between the separating hyperplane and the connecting line l be close to either one of those examples? Or, should the intersection be as far from both points as possible? An intuitive answer is "yes" to the latter: we want the intersection to be as far away from both points as possible.

Let us define a margin γ as the distance between the decision boundary ($\mathbf{w}^\top\tilde{\mathbf{x}}=0$) and the nearest training example $\tilde{\mathbf{x}}$, of course, (loosely) assuming that the decision boundary classifies most of, if not all, the training examples correctly. This assumption is necessary to ensure that there are at least one correctly classified example on each side of the decision boundary. The above thought experiment now corresponds to an idea of finding a classifier that has the largest margin, i.e., a *max-margin classifier*.

The distance to the nearest positive and negative examples can be respectively written down as

$$d^+ = \frac{\mathbf{w}^\top\tilde{\mathbf{x}}^+}{\|\mathbf{w}\|},$$
$$d^- = -\frac{\mathbf{w}^\top\tilde{\mathbf{x}}^-}{\|\mathbf{w}\|},$$

[20] One major difference between this hinge loss and the log loss is that the former is not differentiable everywhere. Does it mean that we cannot use a gradient-based optimization algorithm for finding a solution that minimizes the empirical cost function based on the hinge loss? If not, what can we do about it? The answer is left to you as a **homework assignment**.

Then, the margin can be defined in terms of these two distances as

$$\gamma = \frac{1}{2}(d^+ + d^-) \tag{1.22}$$
$$= ? \tag{1.23}$$
$$= \frac{1}{2\|\mathbf{w}\|}(\mathbf{w}^\top \tilde{\mathbf{x}}^+ - \mathbf{w}^\top \tilde{\mathbf{w}}^-) \tag{1.24}$$
$$= ? \tag{1.25}$$
$$= \frac{1}{2\|\mathbf{w}\|}(C + C) \tag{1.26}$$
$$= \frac{C}{\|\mathbf{w}\|}, \tag{1.27}$$

where C is the unnormalized distance to the positive and negative examples from the decision boundary. These two examples are equi-distance C away from the decision boundary, because our thought experiment earlier suggests that the decision boundary with the maximum margin should be as far away from both of these examples as possible.[21]

Eq. (1.22) states that the margin γ is *inversely proportional* to the norm of the weight vector $\|\mathbf{w}\|$. In other words, we should minimize the norm of the weight vector if we want to maximize the margin.

Support vector machines Now let us put together the hinge loss based empirical cost function and the principle of maximum margin into one optimization problem:

$$J_{\text{svm}}(M, D_{\text{tra}}) = \frac{C}{2} \underbrace{\|\mathbf{w}\|^2}_{\text{(a)}} + \underbrace{\frac{1}{|D_{\text{tra}}|} \sum_{(y,x)\in D_{\text{tra}}} D_{\text{hinge}}(y, \mathbf{x}; M)}_{\text{(b)}}, \tag{1.28}$$

where $C/2$ can be thought of as a regularization coefficient. This is a cost function for so-called support vector machines [2].

This classifier is called a *support vector* machine, because at its minimum, the weight vector can be fully described by a small set of training examples which are often referred to as support vectors. Let us derive it quickly here:

$$\frac{\partial J_{\text{svm}}}{\partial \mathbf{w}} = C\mathbf{w} - \frac{1}{|D_{\text{tra}}|} \sum_{(y,x)\in D_{\text{tra}}} \mathbb{I}(y\mathbf{w}^\top \mathbf{x} \leq 1) y\mathbf{x} = 0$$
$$\Leftrightarrow \mathbf{w} = \frac{1}{C|D_{\text{tra}}|} \sum_{(y,x)\in D_{\text{misclas}}} y\mathbf{x},$$

where D_{miscla} is a set of misclassified, or barely classified, training examples, and

$$\mathbb{I}(a) = \begin{cases} 1, & \text{if } a \text{ is true} \\ 0, & \text{otherwise} \end{cases}.$$

[21] **Homework assignment**: Fill in the missing equations marked by ? in Eq. (1.22), and explain in words the derivation.

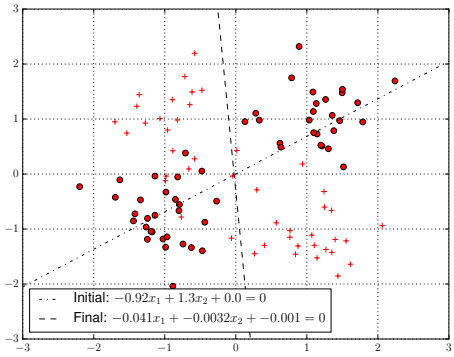


Figure 1.4: If the problem is not linearly separable as in the case shown, a linear classifier, such as perceptron, fails miserably. This is a famous example of a exclusive-or (XOR) problem (with noise.)

Often, $|D_{\text{miscla}}| \ll |D_{\text{tra}}|$, and thus, a support vector machine is categorized into a family of sparse classifiers.

Support vector machines are perhaps the most widely used classifiers since its introduction in early 90's. This is evident from more than 20k citations [2] has gathered since then. some historical account and why we won't be able to cover it more in depth.

1.6 Multi-Class Classification

Perhaps focus only on multi-class logistic regression, i.e., softmax classifier

1.7 Nonlinear Classification

So far in this course, we have looked at a linear classifier which defines a hyperplane ($\mathbf{w}^\top \tilde{\mathbf{x}} = 0$) that partitions the input space into two partitions. Clearly this type of classifier can only solve linearly separable problems. A famous example in which a linear classifier fails is exclusive-OR (XOR) problem shown in Fig. 1.4. In this section, we discuss how to build a classifier for problems which are not linearly separable.

1.7.1 Deep Learning: Adaptive Basis Networks

Feature Extraction

Adaptive Basis Networks and Representation Learning

1.7.2 k-Nearest Neighbours

Radial Basis Function Networks

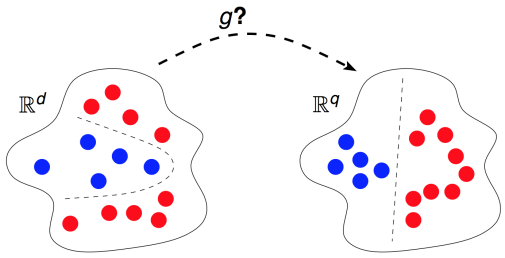


Figure 1.5: The goal of adaptive basis networks is to find a parametrized mapping from the original input space $\mathbf{x} \in \mathbb{R}^d$ to another space $g(\mathbf{x}) \in \mathbb{R}^q$ that makes the problem linearly separable.

k-Nearest Neighbours

1.8 Kernel Support Vector Machines*

1.9 Decision Tree*

1.10 Ensemble Methods*

Chapter 2

Regression

We have so far considered a problem of classification, where the output of a machine M is constrained to be a finite set of discrete labels/classes. In this section, we consider a *regression* problem in which case the machine outputs an element from an infinite set.[1] A general setup of the problem remains largely identical to that from Sec. 1.1, meaning that it is probably a good idea to re-read the section at this point. In the context of regression, we will particularly focus on framing the whole problem as probabilistic modelling.

2.1 Linear Regression

2.1.1 Linear Regression

2.1.2 Regularization and Prior Distributions

2.2 Bayesian Linear Regression and Gaussian Process Regression

2.2.1 Bayesian Approach to Machine Learning

2.2.2 Gaussian Process Regression*: Weight-Space View

[1] This definition however is not universal, in that even when the output is from a finite set, the problem is sometimes called regression if there exists natural ordering of labels.

Chapter 3

Dimensionality Reduction

3.1 Unsupervised Learning: Problem Setup

Unsupervised learning is a weird, but fascinating problem. Unlike supervised learning in which a machine was defined as a transformation of an input vector $\mathbf{x}$, a machine M in unsupervised learning *scores* an input vector according to how likely that vector is. If an input vector $\mathbf{x}$ is likely, the output of the machine $M(\mathbf{x})$ would be higher, and otherwise lower. The use of the term *score* should remind you of our earlier discussion on classification, and it is only natural because there is a strong connection between supervised learning and unsupervised learning. This connection is apparent when we consider $\mathbf{x}$ as a concatenation of an input vector $\mathbf{x}$ and its corresponding label y. Then, with a machine M trained by unsupervised learning, we can classify any given input vector by

$$\hat{y} = \arg\max_{y} M([\mathbf{x}; y]).$$

We can similarly perform regression in this framework.

This capability of scoring an input vector allows us to use it for *outlier detection* as well. Given an input vector $\mathbf{x}$, we will declare it as an outlier if its score is lower than a certain, predefined threshold:

$$\mathbf{x} \text{ is an outlier if } M(\mathbf{x}) < \tau.$$

The threshold τ may be found by any of the validation techniques we discussed in Sec. 1.4.2. Furthermore, we can even *generate* a novel input vector by finding an input vector that maximizes the score given by the model:

$$\hat{\mathbf{x}} = \arg\max_{\mathbf{x}} M(\mathbf{x}).$$

3.1.1 Naive Bayes Classifier

3.2 Dimensionality Reduction: Problem Setup

3.3 Principal Component Anslysis

3.3.1 Maximum Variance Criterion

3.3.2 Minimum Reconstruction Criterion

3.3.3 Probabilistic Principal Component Analysis

Expectation-Maximization Algorithm

3.4 Other Dimensionality Reduction Techniques*

Chapter 4

Clustering

Chapter 5

Structured Output Prediction and Reinforcement Learning

5.1 Time-Series Modelling*

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