CS 337: Artificial Intelligence

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§1. Introduction

1.1. What and Why?

Machine learning involves learning from past experiences to perform a job better.
Broadly, the goal of the field is to make a computer emulate human pattern recognition, which is second nature to us. What do each of these words mean in the context of computer science? "Learning" and "better" usually depend heavily on the context surrounding our goals, and past experiences usually refers to a data set of some form. Broadly, there are two types of learning: *supervised* and *unsupervised*.

In the former, we have access to some **training data**, usually consisting of a set of pairs of input and output. The supervised learning algorithm then analyzes this data to produce an inferred function, which can then be used for determining what unknown inputs (not in the training data) must map to. This requires the algorithm to go from a smaller set of training data to a much broader set of inputs in a way that "makes sense". For example, given the heights and weights of a thousand people, we might be asked to determine the weight of a person of a person of some new height.
In unsupervised learning on the other hand, we do not have access to any prior information, so we must classify them in some sensible manner. For example, given a set of fruits, we may wish to classify them into various groups. If we divide on the basis of colour (alone), we might get two groups – apples and cherries in one and oranges and peaches in the other. If we divide on the basis of both colour and size, we might further divide the first of these groups into two. The computer is forced to create some compact internal representation of the features of these fruits, and from this we might even be able to generate *new* fruits.

How does all this work? It might be simpler to grasp if we dive headlong into an example.
Suppose we are given a data set $\mathcal{D} = \{\langle x_1, y_1\rangle, \ldots, \langle x_k, y_k\rangle\}$. We wish to determine a function f^* such that $f^*(x)$ is the best "predictor" of y with respect to $\mathcal{D}$.
To quantify how good a prediction is, we introduce an *error function* $\varepsilon(f, \mathcal{D})$ that reflects the discrepancy of the function with respect to $\mathcal{D}$. We also assume that our f^* is taken from some base class of functions, say $\mathcal{F}$. We then set

$$f^* = \arg\min_{f \in \mathcal{F}} \varepsilon(f, \mathcal{D}).$$

Typically, we present our function in terms of some "basis functions" $(\phi_i)_{i=1}^n$ each from the set of inputs to $\mathbb{R}$. More compactly, we have a single function ϕ from the set of inputs to $\mathbb{R}^n$ that shows all the relevant things we can glean about any input. Suppose our set of outputs is in $\mathbb{R}^k$. We then learn a function $f : \mathbb{R}^n \to \mathbb{R}^k$ and given a new input x', we predict the corresponding output as $y' = f(\phi(x'))$.
Due to this, it is often helpful to think of the input as an element of $\mathbb{R}^n$, where n is the number of basis functions.

Remark. It is important to note that even though our original input x may be in $\mathbb{R}$, we could have more than just 1 basis function. For instance, we could choose the basis functions as $\{(x \mapsto x^i) : 1 \le i \le 100\}$. This is especially important in the coming topic of linear regression, where linearity in the basis functions should not be mixed up with linearity in the original input.

1.2. Linear Regression

We first discuss perhaps the simplest example of machine learning. In this, the class $\mathcal{F}$ of functions we consider is merely the class of all linear functions over the basis functions. That is,

$$\mathcal{F} = \{(x \mapsto w^\top \phi(x)) : w \in \mathbb{R}^n\}.$$

Observe that if one of our basis functions is 1 (or some constant), this is equivalent to the set of all *affine* functions (linear functions plus a constant).

1.2.1. The method of least squares

Suppose our data set is $\mathcal{D} = \{\langle x_i, y_i \rangle : 1 \le i \le m\}$, where each y_i is in $\mathbb{R}$. In the method of least squares, our choice of error function is given by

$$\varepsilon(f, \mathcal{D}) = \sum_{i=1}^{m} (f(x_i) - y_i)^2.$$

The squared difference is an extremely common error function for various reasons – it is convex, non-negative, and well-behaved.
In the case of linear regression, where any function f is uniquely determined by a $w \in \mathbb{R}^n$, we can express the error in terms of this vector as

$$\varepsilon(w) = \sum_{i=1}^{m} (w^\top \phi(x_i) - y_i)^2.$$

Now, set

$$\Phi = \begin{pmatrix} \phi_1(x_1) & \cdots & \phi_n(x_1) \\ \vdots & \ddots & \vdots \\ \phi_1(x_m) & \cdots & \phi_n(x_m) \end{pmatrix} \text{ and } y = \begin{pmatrix} y_1 \\ \vdots \\ y_m \end{pmatrix}.$$

So,

$$\varepsilon(w) = \|\Phi w - y\|_2^2.$$

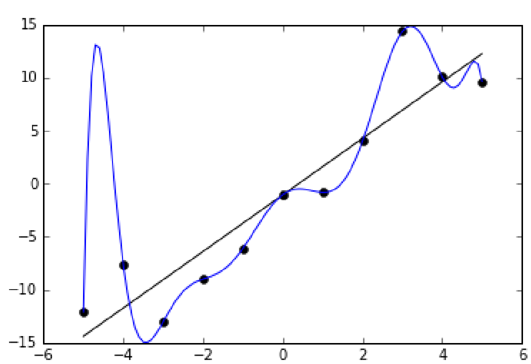
The minimum value of the above is just the distance from y to $\mathcal{C}(\Phi)$, the column space of Φ! Let $\hat{w} = \arg\min_w \varepsilon(w)$. In particular, if $y \in \mathcal{C}(\Phi)$, it is possible to get the cost to 0.
The least square solution is then the distance from y to the projection $\hat{y}$ of y on $\mathcal{C}(\Phi)$. How do we find $\hat{y}$ and $\hat{w}$?
The line joining y and $\hat{y}$ is orthogonal to $\mathcal{C}(\Phi)$. As a result, $(\hat{y} - y)^\top \Phi = 0$. Therefore,

$$\begin{aligned} \hat{y}^\top \Phi &= y^\top \Phi \\ (\Phi \hat{w})^\top \Phi &= y^\top \Phi \\ \hat{w} &= (\Phi^\top \Phi)^{-1} \Phi^\top y. \end{aligned}$$

This is well-defined only if $(\Phi^\top \Phi)$ is invertible (Φ has full column rank).

Remark (Overfitting). One might think that more basis functions means a better approximation. Indeed, this would mean that we have more "freedom", which should allow us to get a better function. However, this is not the case. While adding more basis functions allows us to emulate the *training* data better, we might mimic it too closely and lose sight of the overall behaviour, which results in bad performance when it comes to the general *testing* data.
This is very clearly seen in the following example where the output is slightly noisy linear data, and we have taken two cases: one wherein the basis function are just $\phi(x) = (1, x)$ (fitting a degree 1 polynomial), and the second where $\phi(x) = (1, x, \ldots, x^{10})$ (fitting a degree 10 polynomial).

FIGURE 1 – Overfitted data



1.3. Probabilistic Interpretations

Let us jump away from regression for a moment and look at what happens if instead of trying to learn a function with inputs and outputs, we are instead trying to determine the parameters of some random variable given some datapoints drawn from it.
To do this, suppose that any observation z is drawn from the random variable Z with probability density/mass function g_θ (depending on the parameter θ, which we are trying to learn). For example, if Z is a gaussian with mean μ and variance σ^2, we might have $\theta = (\mu, \sigma^2)$ and

$$g_\theta(z) = \frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{1}{2}\frac{(x-\mu)^2}{\sigma^2}\right).$$

1.3.1. Maximum likelihood estimation

Suppose we are given a dataset $\mathcal{D} = \{z_1, \ldots, z_m\}$.
Also suppose that we have discrete outputs for the moment (g_w is a probability *mass* function). Then, define the **likelihood** function

$$\mathcal{L}(\mathcal{D} \mid \theta) = \Pr[\mathcal{D} \mid \theta].$$

Making the mild assumption that the various datapoints in $\mathcal{D}$ are drawn iid, this can be rewritten as

$$\mathcal{L}(\mathcal{D} \mid \theta) = \prod_{i=1}^{m} g_\theta(z_i).$$

Even in the case where we have a continuous output (so a probability density function) instead, this expression remains the same.
As might be expected, in *maximum likelihood estimation* (MLE), we choose that w which maximizes the likelihood. Often, we work with the *log*-likelihood ℓ as well, which is just defined by $\ell(\mathcal{D} \mid w) = \log \mathcal{L}(\mathcal{D} \mid w)$.

1.3.2. Bayesian estimation

In all that we have done so far, we have arrived at a single estimate for w or θ. However, this may not necessarily be the best option – might it not be better to arrive at a probability distribution for w which represents how likely various values are?
Bayesian estimation is one simple way of doing this.

We make the assumption initially that θ is drawn from some **prior** probability distribution p. Given the dataset $\mathcal{D} = \{z_1, \ldots, z_m\}$ (and the function g_θ from earlier), we try to improve on this prior to get to a **posterior** probability distribution that better reflects how θ behaves, now that we have knowledge about the dataset. To do this, we use Bayes' law:

$$\begin{aligned}\Pr[\theta \mid \mathcal{D}] &= \frac{\Pr[\mathcal{D} \mid \theta]\Pr[\theta]}{\Pr[\mathcal{D}]} \\ &= \frac{\Pr[\mathcal{D} \mid \theta] p(\theta)}{\int \Pr[\mathcal{D} \mid \alpha] p(\alpha)\, \mathrm{d}\alpha}. \end{aligned} \tag{1.1}$$

Note the contrast between this and MLE; in the the former we use $\Pr[\theta \mid \mathcal{D}]$, whereas in the latter we use $\Pr[\mathcal{D} \mid \theta]$.
We can then use the posterior to return some estimate of θ.
In *maximum a posteriori estimation* (MAP estimation), we return the mode of the posterior density.
In *Bayesian estimation*, we return the mean of the posterior density.
In the pure Bayesian estimate, we do not return any point estimate for θ at all, and we instead use Bayes' rule to calculate the output given an input as

$$\Pr[x \mid \mathcal{D}] = \int p(x \mid \theta) p(\theta \mid \mathcal{D})\, \mathrm{d}\theta$$

Now, the integral in the denominator of (1.1) can be quite daunting. To deal with this, we introduce the idea of a **conjugate prior**. Such a prior is of the form that the base distribution of both the prior and the posterior are the same. This then enables us to skip the calculation of the denominator, since it merely leads to a constant to normalize the distribution (its integral must be 1), and we know this constant from the structure of the distribution anyway. This can be better understood by an example. Suppose that the datapoints are drawn from a Bernoulli distribution with parameter θ. We then have

$$\Pr[\mathcal{D} \mid \theta] = \theta^r (1-\theta)^{m-r},$$

where r is the number of 1s in $\mathcal{D}$. If we choose our prior to be a Beta distribution with parameters α and β, then the numerator of (1.1) is

$$\theta^r (1-\theta)^{m-r} \cdot \theta^{\alpha-1}(1-\theta)^{\beta-1} \frac{\Gamma(\alpha)\Gamma(\beta)}{\Gamma(\alpha+\beta)}.$$

This is proportional to $\theta^{\alpha+r-1}(1-\theta)^{m-r+\beta-1}$. Since the denominator only gives a constant multiplicative factor, the posterior must just be $\mathrm{Beta}(\alpha+r, \beta+m-r)$.

Some more examples are that the Dirichlet distribution is the conjugate prior to the multivariate Bernoulli and the Gaussian is the conjugate prior to the Gaussian.
Bayesian estimation takes care of overfitting

1.3.3. Relating probabilistic interpretations and regression

Let us jump back to regression. While we typically assume that our input/output pairs are initially taken from some basic (fixed) function f, this is typically not the case. Indeed, we usually have some amount of error when taking the observations itself. This error is commonly taken to be a Gaussian with 0 mean and some (small) variance σ^2. The output as a whole is then just a random variable, with the parameters involving our base parameter θ *and* the input.

For example, let our training data set be $\mathcal{D} = \{\langle x_1, y_1\rangle, \ldots, \langle x_m, y_m\rangle\}$ where the x_i are in $\mathbb{R}^n$ and the y_i in $\mathbb{R}$. Let us perform normal linear regression, but also add a Gaussian error of known variance σ^2. That is, if the input is x, we predict the distribution of the corresponding output y to be $\mathcal{N}(w^\top x, \sigma^2)$.
Supposing we use MLE, we wish to determine

$$\hat{w} = \arg\max_w \frac{1}{(\sqrt{2\pi}\sigma)^m} \exp\left(-\frac{1}{2\sigma^2}\sum_{i=1}^m (y_i - w^\top x_i)^2\right).$$

It is not too difficult to see that this is in fact the same solution as that given by the discussion in the method of least squares.

1.4. Regularisation

As mentioned in a remark towards the end of Section 1.2.1, overfitting tends to make the error over the test data too large, due to large fluctuations in the model we learn (to emulate the training data better). However, this also leads to large coefficients of the learnt vector, and thus large norm. Regularisation attempts to fix this, by further adding in the constraint that $\|w\|_2$ is not too large.

This leads to the *penalized regularised least squares regression problem*, where the cost function is replaced with

$$\|\Phi w - y\|_2^2 + \lambda\Omega(w).$$

We are said to be performing

- *ridge regression* if $\Omega(w) = \|w\|_2^2$,
- *lasso regression* if $\Omega(w) = \|w\|_1$, and

- *support-based penalty regression* if $\Omega(w) = \|w\|_0$.[1]

The closed-form solutions to the first two can be computed by setting the gradient to 0. In particular, the closed-form solution for ridge regression is

$$\hat{w} = (\Phi^\top \Phi + \lambda I)^{-1} \Phi^\top y.$$

Also, this in fact corresponds to performing Bayes/MAP estimation with a multivariate Gaussian prior of mean 0 and variance $(1/\lambda)I$.

Alternatively, we have the *constrained regularised least squares regression problem*, where the cost function is the normal $\|\Phi w - y\|_2^2$, but we have the added constraint that $\Omega(w) \leq \theta$ for some fixed θ.
We again have ridge, lasso, or support-based penalty regression depending on Ω.
It in fact turns out that the above two constraints are equivalent – for any penalized formulation with a λ, there is a corresponding constrained formulation problem with some θ, and vice-versa.

Why is lasso regression interesting? Observe that the level curves of $\|w\|_1$ (namely cross-polytopes) have many corners, and as a result, it is likely that many components of w are close to 0. That is, the learnt vector is likely very sparse, which is desirable.

[1] Here, $\|w\|_0$ is equal to the number of non-zero components.