Differential Description Length for Hyperparameter Selection in Machine Learning

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This paper introduces a new method for model selection and more generally hyperparameter selection in machine learning. The paper first proves a relationship between generalization error and a difference of description lengths of the training data; we call this difference differential description length (DDL). This allows prediction of generalization error from the training data alone by performing encoding of the training data. This can now be used for model selection by choosing the model that has the smallest predicted generalization error. We show how this encoding can be done for linear regression and neural networks. We provide experiments showing that this leads to smaller generalization error than cross-validation and traditional MDL and Bayes methods.

1 Introduction

Minimum description length (MDL) is an established method for model selection. It was developed in the pioneering papers by Rissanen (1978, 1983, 1986), and has found wide use (Grunwald, 2007).

The aim of the current paper is to extend description length methodology (which we use as a broader term than MDL) to model selection for practical machine learning methods. We consider a supervised learning problem with features $x$ and labels $y$. Given a set of training data $(x^n, t^n)$ we want to find a predictor $f(x; \theta_h, h)$ of $y$. Here $\theta_h$ is a a set of parameters that are estimated from the training data, and $h$ is a set of hyperparameters that are chosen; these are typically the model order, e.g., number of hidden units and layers in neural networks, but also quantities like regularization
parameters and early stopping times (Bishop 2006). The goal is to minimize the test error, or generalization error,

\[ E[L(y, f(x; \theta_h, h))] \] 

for some loss function \( L \). However, only the empirical loss (risk) is available:

\[ \frac{1}{n} \sum_{i=1}^{n} L(t_i, f(x_i; \theta_h, h)) \] 

Purely minimizing the empirical loss with respect to the hyperparameters \( h \) can lead to overfitting (Bishop 2006; Hastie et al. 2009). Description length is one method to avoid this.

Using MDL for model selection in learning has been considered before, e.g., Grünwald (2011); Watanabe (2013); Watanabe & Roos (2015); Kawakita & Takeuchi (2016); Alabdulmohsin (2018). In this paper we directly relate a type of description length and generalization error (Theorem 1), using the principles of Fogel & Feder (2018), and this provides a strong rationale for using description length for learning. We then use this theory to develop practical methods for model selection, in particular in neural networks and deep learning.

2 Theory

We consider a supervised learning problem with features \( x \) and labels \( y \). The data \( (x, y) \) is governed by a probability law \( P_\theta(y|x)p(x) \), where \( \theta \) is a parameter vector; these can be probability mass functions or probability density functions. Notice that the distribution of the features \( x \) does not depend on \( \theta \).

We are given a training set \( \{(x_i, t_i), i = 1, \ldots, n\} \) which we assume is iid from the distribution \( P_\theta(y|x)p(x) \). We use the notation \( (x^n, t^n) \) to denote the whole training set. The problem we consider is, based on the training data, to estimate the probability distribution \( \hat{P}_L(y|x) \) so as to minimize the log-loss or cross-entropy

\[ E_\theta [-\log \hat{P}_L(y|x)]. \] 

The expectation here is over both test data and the training set, \( \{(x, y); (x^n, t^n)\} \), with respect to the distribution \( P_\theta(y|x)p(x) \), for a fixed \( \theta \). We will discuss other loss functions later.

2.1 Universal Source Coding and Learning

In this section we assume that the data is from a finite alphabet. Based on the training data \( (x^n, t^n) \) we want to find a good estimated probability law \( \hat{P}_L(y|x) \), which need not be of the type \( P_\theta(y|x) \), and consider as in (3) the log-loss

\[ C_L(n, \hat{P}, \theta) = E_\theta \left[-\log \hat{P}_L(y|x)\right] \] 

Importantly, we can interpret \( C_L(n, \hat{P}, \theta) \) as a code length as follows. By a code length we mean the number of bits required to represent the data without loss (as when
zipping a file). First the encoder is given the training data \((x^n, t^n)\) from which it forms \(P(y|x)\); this is shared with the decoder. Notice that this sharing is done ahead of time, and does not contribute to the codelength. Next, the encoder is given new data \((x^m, y^m)\). The decoder knows \(x^m\) but not \(y^m\). The encoder encodes \(y^m\) using \(\hat{P}_L(y|x)\) (using an algebraic coder \([\text{Cover & Thomas} 2006]\)), and the decoder, knowing \(x^m\), should be able to decode \(y^m\) without loss. The codelength averaged over all training and test data is then \(C_L(n, \hat{P}, \theta)\) within a few bits \([\text{Cover & Thomas} 2006]\). Since this is based on training data, we call this the learned codelength.

The goal is minimize the codelength \(C_L(n, \hat{P}, \theta)\), equivalently the log-loss. The codelength depends on the true probability distribution, i.e., \(\theta\), but we would like an estimator \(\hat{P}\) that is reasonably good for all \(\theta\). In order to do so we first define the regret (or redundancy) of an estimator as

\[
R_L(n, \hat{P}, \theta) = E_{\theta} \left[ -\log \hat{P}_L(y|x) \right] - E_{\theta} \left[ -\log P_{\theta}(y|x) \right]
\]

\[
= E_{\theta} \left[ -\log \hat{P}_L(y|x) \right] - H_{\theta}(Y|X)
\]

\[
= D(P_{\theta} \parallel \hat{P}_L),
\]

(5)

where \(H_{\theta}(Y|X)\) is the conditional entropy and \(D(P_{\theta} \parallel \hat{P}_L)\) is the relative entropy or Kulbach-Leibner distance \([\text{Cover & Thomas} 2006]\). The regret is the difference in codelength between the trained coder and a omniscient coder/decoder knowing the actual value of \(\theta\). Minimizing codelength is equivalent to minimizing regret. A reasonable goal is to minimize the worst case regret over all \(\theta\), and we therefore define the optimum estimator as

\[
\hat{P}_{L,\text{opt}} = \arg \min_{\hat{P} \in \mathcal{P}} \sup_{\theta} R_L(n, \hat{P}, \theta),
\]

where \(\mathcal{P}\) is some set, and correspondingly the minimax regret

\[
R_L^+(n) = \min_{\hat{P} \in \mathcal{P}} \sup_{\theta} R_L(n, \hat{P}, \theta).
\]

We now define

\[
C_L^+(n, \theta) = R_L^+(n) + H_{\theta}(Y|X).
\]

This can be considered the average codelength when the distribution of data is given by \(P_{\theta}(y|x)\) and the coding distribution \(\hat{P}_{L,\text{opt}}\) is used. This is similar to the problem setup considered in \([\text{Fogel & Feder} 2018]\).

A related problem to the above is universal coding of the training data itself. In this case we assume the decoder knows the features \(x^n\) in the training data but not the corresponding labels \(t^n\); the task is to communicate these to the decoder. Again, we want to find a good estimated probability law \(\hat{P}_U(y|x)\) and consider the universal codelength

\[
C_U(n, \theta) = E_{\theta} \left[ -\log \hat{P}_U(t^n|x^n) \right]
\]

(6)

The expectation here is over the training data only. Notice that in this case, as opposed to learned codelength, the decoder does not know which \(\hat{P}_U(y|x)\) the encoder is using,
Figure 1: Universal and learned coding. In learned coding the decoder knows the coding distribution $\hat{P}$. Here $C_U(n, \theta)$ and $mC_L(n, \theta)$ are the number of bits transmitted from encoder to decoder. Dashed lines indicate side-information.

and some bits are therefore needed to encode this information, either explicitly or implicitly. This is a key difference with learned coding, see Fig. 1. Similarly to (5) we define the regret

$$R_U(n, \hat{P}, \theta) = E_\theta \left[ -\log \hat{P}_U(t^n|x^n) \right] - E_\theta \left[ -\log P_\theta(t^n|x^n) \right]$$

$$= E_\theta \left[ -\log \hat{P}_U(t^n|x^n) \right] - nH_\theta(Y|X)$$

(by the iid assumption $P_\theta(t^n|x^n) = \prod_{i=1}^n P_\theta(t_i|x_i)$) and

$$R_U^+(n) = \min_{\hat{P} \in \mathcal{P}} \sup_{\theta} R_U(n, \hat{P}, \theta)$$

$$\hat{P}_{U, \text{opt}} = \arg \min_{\hat{P} \in \mathcal{P}} \sup_{\theta} R_U(n, \hat{P}, \theta)$$

$$C_U^+(n, \theta) = R_U^+(n) + nH_\theta(Y|X)$$

(7)

Again, we can interpret $C_U^+(n, \theta)$ as the average codelength to encode $t^n$ when the distribution of data is given by $P_\theta(y|x)$ and the coding distribution $\hat{P}_{U, \text{opt}}$ from (7) is used. This is a problem that has a long history in universal source coding, e.g., Shamir (2006). A difference from traditional universal source coding is that there are features $x^n$ known to both encoder and decoder, but this does not change the problem fundamentally. Therefore, many results from universal source coding can be used. Given a specific training sequence $(x^n, t^n)$ we can use a universal source coding algorithm (Shamir 2006) to encode $t^n$, denoting the resulting codelength $\hat{C}_U(n)$ (which depends on the specific $(x^n, t^n)$). For a good source coder we have

$$\hat{C}_U(n) \approx C_U^+(n, \theta)$$
Thus, although $C_U^-(n, \theta)$ might not be known, we can find good estimates.

The main result of the paper is the following theorem relating learned coding and universal source coding:

**Theorem 1.** Assume that the set of distributions $\mathcal{P}$ is compact and convex. Then the learned codelength is bounded by

$$C_L^+(n, \theta) \leq C_U^+(n+1, \theta) - C_U^+(n, \theta)$$

**Proof.** An alternative way to think of the problem is that there is an unknown prior $w$ over $\theta$. We can then define

$$\hat{R}_L^+(n) = \min_{P \in \mathcal{P}} \sup_{w} E_w[R_L(n, \hat{P}, \theta)]$$

$$\tilde{R}_L^-(n) = \sup_{w} \min_{P \in \mathcal{P}} E_w[R_L(n, \hat{P}, \theta)]$$

It is clear that $\tilde{R}_L^-(n) \leq R_L^+(n) \leq \hat{R}_L^+(n)$. We can write the expectation explicitly as

$$E_w[R_L(n, \hat{P}, \theta)] = \int w(\theta) D(P_\theta \parallel \hat{P}) d\theta$$

This is concave (linear) in $w$ and convex in $\hat{P}$ (Cover & Thomas, 2006) and the optimization is over compact sets. Therefore, by the minimax theorem (Von Neumann, 2007), $\tilde{R}_L^-(n) = R_L^+(n) = \hat{R}_L^+(n)$.

Similarly, for universal source coding $\tilde{R}_U^-(n) = R_U^+(n) = \hat{R}_U^+(n)$, which is a well-known fact (Shamir, 2006).

To find the universal codelength $R_U^+(n)$ we need to find an optimum coding distribution for a given prior $w$. This is the same as the optimum Bayes estimator (Scharf, 1990), which is given by

$$\hat{P}_U(t^n|x^n) = \int P_\theta(t^n|x^n) w(\theta) d\theta$$

For learned coding, the expectation is over the training $(x^n, t^n)$ and the single test data $(x, y)$; we can append the $x$ to $x^n$ and denote this by $x^{n+1}$. The optimum coding distribution for the learned codelength $R_L^+(n)$ is given by Bayes rule

$$\hat{P}_L(y|x; \{x^n, t^n\}) = \frac{P(y, x, x^n, t^n)}{P(x^{n+1})}$$

where the joint probability distributions are

$$P(y, x, x^n, t^n) = \int P_\theta((y, t^n)|x^{n+1}) P(x^{n+1}) w(\theta) d\theta$$

$$= P(x^{n+1}) \int P_\theta((y, t^n)|x^{n+1}) w(\theta) d\theta$$

$$= P(x^{n+1}) \hat{P}_U((y, t^n)|x^{n+1})$$

The fact that there are features in addition to labels does not make an essential difference.
\[ P(x, x^n, t^n) = \int P_\theta(t^n|x^{n+1})P(x^{n+1})w(\theta)d\theta \]
\[ = P(x^{n+1}) \int P_\theta(t^n|x^n)w(\theta)d\theta \]
\[ = P(x^{n+1})P_U(t^n|x^n) \]

Thus
\[ \hat{P}_L(y|x; \{ x^n, t^n \}) = \frac{\hat{P}((y, t^n)|x^{n+1})}{\hat{P}_U(t^n|x^n)} \]

Then for a given prior \( w \) and true parameter \( \theta \) we have
\[
R_L(n, w) = \sum_{x^{n+1}, t^n, y} -P((y, t^n), x^{n+1}) \log \hat{P}_L(y|x; \{ x^n, t^n \}) \\
- E_w[H_\theta(Y|X)] \\
= \sum_{x^{n+1}, t^n, y} -P((y, t^n), x^{n+1}) \log \hat{P}((y, t^n)|x^{n+1}) \\
- (n + 1)E_w[H_\theta(Y|X)] \\
- \left( \sum_{x^n, t^n} -P(t^n, x^n) \log \hat{P}_U(t^n|x^n) - nE_w[H_\theta(Y|X)] \right) \\
= R_U(n + 1, w) - R_U(n, w) \\

\]

For the first term here we consider \( t^n, y \) as combined training data \( t^{n+1} \). Now
\[
C_L^+(n, \theta) = R_L^+(n) + H_\theta(Y|X) = \hat{R}_L^-(n) + H_\theta(Y|X) \\
= \sup_w R_L(n, w) + H_\theta(Y|X) \\
= \sup_w R_U(n + 1, w) - R_U(n, w) + H_\theta(Y|X) \\
\leq \sup_w R_U(n + 1, w) + (n + 1)H_\theta(Y|X) \\
- \left( \sup_w R_U(n, w) + nH_\theta(Y|X) \right) \\
= C_U^+(n + 1, \theta) - C_U^+(n, \theta) \\

\]

The importance of the theorem is that it allows us to find learned codelength (i.e., generalization error) in terms of universal codelength. To find generalization error directly, one would need additional data, whereas the universal codelength is a property of the training data itself.
2.2 Use for model selection

Consider selection between two models $\mathcal{M}_1$ and $\mathcal{M}_2$ with probability laws $P_{1,\theta_1}(y|x)$ and $P_{2,\theta_2}(y|x)$. A model selection rule is a decision rule $\phi : \mathcal{X}^n \times \mathcal{Y}^n \to \{1, 2\}$. For a specific decision rule, let $p_{ji}(\theta_i, P_j)$ be the probability of choosing model $j$ when model $i$ is true, which in general depends on $\theta_i$ as well as the distribution $P_j$ of the features $x$. Suppose that the data is generated by model $i$ and that $\phi$ chooses the correct model. The generalization error for log-loss is then given by (5) as $D(P_{1,\theta_1} \parallel P_{1,\hat{\theta}_1})$. If $\phi$ chooses the wrong model, the generalization error is $C_L(n, P_{2,\hat{\theta}_2}, \theta_1)$ and the regret by (5) as $D(P_{1,\theta_1} \parallel P_{2,\hat{\theta}_2})$. We define the conditional regret of $\phi$ as

\[
R_1 = \sup_{\theta_1, p_x} \left\{ p_{11}(\theta_1, p_x)C_L(n, P_{1,\theta_1}, \theta_1) \right. \\
+ p_{21}(\theta_1, p_x)C_L(n, P_{2,\hat{\theta}_2}, \theta_1) - H_{\theta_1}(Y|X) \right\}
\]

\[
R_2 = \sup_{\theta_2, p_x} \left\{ p_{22}(\theta_2, p_x)C_L(n, P_{2,\theta_2}, \theta_2) \right. \\
+ p_{12}(\theta_2, p_x)C_L(n, P_{1,\hat{\theta}_1}, \theta_2) - H_{\theta_2}(Y|X) \right\}
\]

That is, $R_i$ is the regret of $\phi$ when the model is $\mathcal{M}_i$. As in Section 2.1 we consider minimax regret, and an optimum decision rule would minimize the maximum regret, $R = \max\{R_1, R_2\}$, i.e., minimax hypothesis testing ($\text{Scharf [1990]}$). Finding the optimum decision rule is in general impossible, so our goal is to find good practical decision rules. However, one can notice that usually optimum minimax detectors have $R_1 = R_2$ ($\text{Scharf [1990]}$), so a good decision rule should have $R_1 \approx R_2$.

Specifically, we will develop decision rules based on the theory in Section 2.1. A reasonable decision rule is to choose the model that has the smallest predicted generalization error. There is of course no guarantee it will lead to optimum minimax performance. Since the generalization error can be bounded by the differential description length by Theorem 1, one could use the rule

\[
m = \arg \min \{ \hat{C}_{1,U}(n) - \hat{C}_{1,U}(n-1), \hat{C}_{2,U}(n) - \hat{C}_{2,U}(n-1) \},
\]

where $\hat{C}_{1,U}$ is the length of the output of a universal source coder for model $\mathcal{M}_i$.

We call $\hat{C}_{1,U}(n) - \hat{C}_{1,U}(n-1)$ differential description length (DDL).

The issue with using (9) directly is that $\hat{C}_{1,U}(n)$ is a noisy estimate of $C_{1,U}^+(n, \theta)$, and that $\hat{C}_{1,U}(n) - \hat{C}_{1,U}(n-1)$ as a difference of two noisy estimates therefore is quite inaccurate. We instead suggest to use $\hat{C}_{1,U}(n) - \hat{C}_{1,U}(n-n_t)$ for some integer $n_t$,

\[
m = \arg \min \{ \hat{C}_{1,U}(n) - \hat{C}_{1,U}(n-n_t), \hat{C}_{2,U}(n) - \hat{C}_{2,U}(n-n_t) \}. \tag{10}
\]
We can write \( \hat{C}_{1,U}(n) - \hat{C}_{1,U}(n - n_t) = \sum_{j=n}^{n-n_t-1} \hat{C}_{1,U}(j) - \hat{C}_{1,U}(j - 1) \), an average of the differential over the last \( n_t \) samples. In experiments we have seen that the performance is quite insensitive to \( n_t \).

We will illustrate how the above rule works on a simple example. The data \((x, y)\) is (iid) binary given by a conditional probability distribution \( P(y|x) \) (and marginal \( P_x(x) \)). Under model \( \mathcal{M}_1 \), \( y \) is independent of \( x \), while under \( \mathcal{M}_2 \) \( y \) is dependent on \( x \). For model \( \mathcal{M}_1 \) there is a single unknown parameter \( \theta_1 = p(1|0) = p(1|1) \), while for \( \mathcal{M}_2 \) there are two unknown parameters \( \theta_2 = (p(1|0), p(1|1)) \). From Shamir (2006) we can conclude that the description length is

\[
\hat{C}_{1,U}(n) = nH(\hat{Y}) + \frac{1}{2} \log n
\]

\[
\hat{C}_{2,U}(n) = nH(\hat{Y}|\hat{X}) + \log n
\]

except for some small terms. Here \( H(\hat{Y}|\hat{X}) \) is the entropy calculated for the empirical distribution of the training data.

Theoretical analysis of even this simple model is very complex, even though we have closed-form expressions (11) for code length, as it is not easy to calculate (8). We will therefore limit ourselves to a numerical maximization over the parameters in (8).

Fig. 2 shows the regret as a function of \( n \) for both full description length (i.e., essentially \( n_t = n \)) and differential description length when \( n_t \) is optimized. As mentioned above, a good decision rule should have \( R_1 \approx R_2 \). For both methods we conclude it seems like \( \frac{R_2(n)}{R_1(n)} = c \), where \( c \) is independent of \( n_t \), which is a reasonable expression of \( R_1 \approx R_2 \). As the main point, we see that the minimax regret is smaller for DDL than for full description length.

![Figure 2: The figure shows worst case generalization error when data is dependent or independent, for either differential description length with optimum \( n_t \) or full description length.](image)

The remaining issue is how to choose \( n_t \). Fig. 3 shows the regret as a function of
The main conclusion is that unless we choose \( n_t \) very small or very large, the exact value has little effect. It seems that a good simple choice could be \( n_t = \frac{n}{2} \).

![Figure 3](image)

Figure 3: The figure shows generalization error versus \( n_t \) when data is dependent or independent for different values of \( n \). The dots are the generalization error for full description length (MDL).

### 3 Hyperparameter Selection in Machine Learning

In order to use description length for machine learning, the machine learning methods need to be able to code data. For example, for discrete labels softmax output used in neural networks can be interpreted as a probability which can be input to an algebraic coder (Cover & Thomas, 2006), and the negative logarithm of the probability therefore can be interpreted as a codelength, within a few bits.

If the alphabet for \( Y \) are the reals, encoding (exactly) requires an infinite number of bits. We can still argue that (4) and (6) are actual codelengths when we use a pdf for \( \hat{P} \) as follows. We will assume a fixed point representation of the reals with a (large) finite number, \( r \), bits after the period, and an unlimited number of bits prior to the period as in Rissanen (1983). Assume that the data is distributed according to a pdf \( f(x) \). Then the number of bits required to represent \( x \) is given by

\[
C = -\log \int_x^{x+2^{-r}} f(t) dt \approx -\log(f(x)2^{-r}) \\
= -\log(f(x)) + r
\]  

(12)

When we use description length, we are only interested in comparing codelengths, so the dependency on \( r \) cancels out.

With the above, in general we can write the codelength to encode training data as

\[
C = -\log P(t^n|x^n; \hat{\theta}_h, h),
\]  

(13)
where $h$ denotes the hyperparameters. This is a codelength, but it requires the decoder to know $\hat{\theta}_h$ (both encoder and decoder are assumed to know $h$). MDL (Rissanen 1978, 1983, 1986; Grunwald 2007) therefore additionally encodes $\hat{\theta}_h$; since encoding the exact value requires an infinite number of bits, instead an approximation $\hat{\theta}_{h,q}$ is encoded, and the total codelength is minimized

$$C_U(n, h) = \min_{\hat{\theta}_{h,q}} -\log P(t^n|x^n; \hat{\theta}_{h,q}, h) + L(\hat{\theta}_{h,q}),$$

(14)

where $L(\hat{\theta}_{h,q})$ is the number of bits required to encode $\hat{\theta}_{h,q}$, which can be either explicit or implicit. The minimizing $\hat{\theta}_{h,q}$ is usually close to the maximum likelihood solution $\hat{\theta}_h$, and $C_U$ can be taken as expressing how well the model fits the given observation.

Now, in machine learning the aim is to minimize generalization error (1), not as such fitting a model. Rather than using MDL directly, we can use it through Theorem 1 by relating generalization error and universal codelength. In this context, $C_U$ in (14) can indeed be thought of as a universal codelength given a certain model class in the sense of Section 2.1, and it can therefore be used in Theorem 1 to estimate generalization error.

With the above, we can now use the theory in Section 2.1. Practically we can use (10) to decide between models, which in terms of hyperparameter optimization can be written as

$$h = \arg \min_{\hat{\theta}_h} \hat{C}_U(n, \hat{h}) - \hat{C}_U(n - n_t, \hat{h})$$

(15)

In this rule, $\hat{C}_U(n, h)$ is the codelength of a universal source coder of the sequence $t^n$. Many universal source coders and MDL methods are sequential, for example Lempel-Ziv (Ziv & Lempel 1977, 1978) and CTW (Willems et al. 1995) and predictive MDL (Rissanen 1986). For such methods, the decoder decodes $t^m$, $m < n$, and uses that information to decode $t_{m+1}$ repeatedly. Therefore the number of bits used to encode $t^m$ is the same whether or not $t^m$ is encoded by itself, or as the beginning of a longer sequence $t^n$. As a consequence, for such methods $\hat{C}_U(n, h) - \hat{C}_U(n - n_t, h) = \hat{C}_U(n|t^{n-n_t}, h)$, where $\hat{C}_U(n|t^{n-n_t}, h)$ is the codelength of encoding $t^n$ when the encoder and decoder are given the side information of $t^{n-n_t}$. The expression $\hat{C}_U(n|t^{n-n_t}, h)$ has the advantages that it is less noisy than $\hat{C}_U(n, h) - \hat{C}_U(n - n_t, h)$, mainly because each term in the difference has its own uncertainty. We will therefore use

$$h = \arg \min_{\hat{h}} \hat{C}_U(n|t^{n-n_t}, h).$$

(16)

This methodology has further advantages, which will be discussed shortly.

The above methodology is specifically aimed at minimizing generalization error in terms of log-loss. This is useful as the log-loss in some sense dominates all other loss functions (Painsky & Wornell 2018) – so, if we minimize the log-loss, other losses will also be kept small. In our experiments we have observed that when we minimize log-loss, in general other loss functions will also be reduced, see for example Fig. 7 later.
When applying the above to machine learning methods, there are several complications. One is that practical machine learning algorithms usually do not/cannot find the globally optimum solution, and the minimization in (14) therefore does not make sense. Rather, for a given set of hyperparameters \( h \) we get a (suboptimum) solution \( \hat{\theta}^*(h) \) (that is, \( \hat{\theta}(h) \) is some particular output of a machine learning algorithm, not necessarily the solution of an optimization problem). To resolve this, we think of a set of hyperparameters giving a solution region \( \Theta(h) \) rather than just a single solution \( \hat{\theta}(h) \) and replace the solution (14) with

\[
C_U = \min_{\hat{\theta}_h,q \in \Theta(h)} -\log P(t^n|x^n; \hat{\theta}_h,q,h) + L(\hat{\theta}_h,q) \tag{17}
\]

For example, \( \hat{\theta}(h) \) might be a local minimum and \( \Theta(h) \) the neighborhood where \( \hat{\theta}(h) \) is the minimum. Thus, \( \hat{\theta}_h,q \) is still a solution to an optimization problem, we can think of (17) as a universal source coder, and as long as \( \Theta(h) \) is convex (we can just take it for example as an \( L_2 \) n-ball around \( \hat{\theta}(h) \)), Theorem 1 applies.

One common set of hyperparameters is regularization parameters. Many regularization functions can be thought of giving a prior on \( \theta_h \), \( P(\theta_h; h) \); for example, \( L_2 \) regularization can be thought of as giving a Gaussian prior on \( \theta_h \). With this, we can write (17) as

\[
C_U = \min_{\hat{\theta}_h,q \in \Theta(h)} -\log P(t^n|x^n; \hat{\theta}_h,q,h)P(\hat{\theta}_h,q; h) + L(\hat{\theta}_h,q) \tag{18}
\]

essentially a MAP (Maximum Aposteriory) solution instead of a maximum likelihood solution, and Theorem 1 therefore still applies.

We focus on MDL methods that are based on actual encoding of data rather than simple approximations of codelength. We do not believe that simple approximate formulas can always capture the complexity of complex learning algorithms. As an example, the impact of regularization parameters are not characterized by simply counting the dimension of the parameter space. There are a number of such methods, for example normalized maximum likelihood (NML) (Shtar’kov 1987), sequential NML (Roos & Rissanen 2008), sufficient statistics (Sabeti & Host-Madsen 2017). In the current paper we limit ourselves to Rissanen’s predictive MDL (Rissanen 1986) that calculates a codelength

\[
C = -\sum_{i=0}^{n-1} \log P(t_{i+1}|x_{i+1}; \hat{\theta}_h(t^i,x^i), h), \tag{19}
\]

where \( \hat{\theta}_h(t^i,x^i) \) is the maximum likelihood estimate. Predictive MDL has the advantage that is straightforward to implement once one has a maximum likelihood solution. But an issue with predictive MDL is initialization: \( \hat{\theta}_h(t^i,x^i) \) is clearly not defined for \( i = 0 \), and likely \( i \) should be large for the estimate to be good. When the initial estimate is poor, it can lead to very long codelengths, see Sabeti & Host-Madsen (2017). Fortunately, DDL completely overcomes this problem when \( C_{1,D}(n) - C_{1,U}(n-n_t) = C_{1,U}(n|x^{n-n_t}) \) is used. Therefore, predictive MDL is a promising method for machine learning.
4 Linear Regression

We will first show how the methodology can be applied to a simple machine learning method, linear regression.

Let \( \Phi_m = [\phi(x_1), \ldots, \phi(x_m)] \), where \( \phi(x_i) \) are the feature vectors. Assuming a Gaussian model with variance \( \beta \), the ML estimate with regularization is (e.g., Bishop (2006); Scharf (1990))

\[
\hat{w}_m = \left( \Phi_m^T \Phi_m + \lambda I \right)^{-1} \Phi_m^T y_m \\
\hat{\beta}_m = \left( \frac{1}{m} \sum_{i=1}^{m} (t_i - \hat{w}_m^T \phi(x_n))^2 \right)^{-1}
\]  

(20)

The estimate (20) is not defined until \( m \) is at least equal to the dimension of the feature space. But even then, the estimate is not reliable, and using this directly for MDL can give a codelength which is nearly infinite, which makes predictive MDL not very useful. However, with DDL implemented through (16) we only need to calculate (20) for \( m \geq n - n_t \), which makes it much more reliable. There are recursive algorithms for updating \( \hat{w}_m \) (Haykin, 2002), so predictive MDL/DDL can be implemented very efficiently.

Figure 4 shows some experimental results. The setup is that of fitting polynomials of order up to 20 to the curve \( \sin(3x) \), \( x \in [-2, 2] \). We generate 500 random \( x_n \) and observe \( t_n = \sin(3x_n) + w_n \), where \( w_n \sim N(0, 0.15) \). We seek to optimize the regularization parameter \( \lambda \) in \( L_2 \) regularization. We use DDL with \( n_t = \frac{n}{4} \) and compare with cross-validation, where we use 25% of samples for cross-validation. We also compare with Bayes model selection, using the theory in Bishop (2006, Section 3.5.1) to optimize \( \alpha = \lambda \hat{\beta} \). We plot the difference from the minimum generalization error when \( \lambda \) is chosen to minimize the actual generalization error (calculated over 50,000 samples), excess generalization error. One can see that DDL essentially chooses the correct \( \lambda \) in nearly 50% of cases, and is always better than cross-validation. It also clearly better than the Bayes method (which, in its defense, was not developed specifically to minimize generalization error). The curves for MSE rather than log-loss are nearly identical, so we have not included them.

In Fig. 5 we modify the experiment to directly varying the model order \( M \) without regularization. In that case we can also compare with traditional MDL (Rissanen, 1983) through the simple approximation of (14) by

\[
C_V(n, h) = \min_{\hat{\beta}_n} \log P(t^n|x^n; \hat{\beta}_h, h) + \frac{M}{2} \log n
\]

We see that DDL is again better than cross-validation, and better than traditional MDL, except that DDL and cross-validation have heavy tails.

\[\text{[2]}\text{The reason cross-validation can have negative excess generalization error is that \( \hat{w} \) is calculated from only 75% of samples, and that has a chance of being better than an estimate calculated from the full set of training samples.}\]
Figure 4: Generalization error for least squares for simple curve fitting with regularization optimization. The curves show the distribution of excess generalization error in terms of the CDF.

5 Neural Networks

MDL theory is based on maximum likelihood solutions, i.e., \( \text{(14)} \). On the other hand, training of a neural network is unlikely to converge to the maximum likelihood solution. Rather, the error function has many local minima, and training generally iterates to some local minimum (or a point near a local minimum), and which one can depend on the initialization condition, i.e., a solution of the type in \( \text{(18)} \). This requires adaption of methods like predictive MDL \( \text{(19)} \). Another challenge is complexity. For example, directly using predictive MDL \( \text{(19)} \) requires training for every subset of samples \((x', t')\) for \( i = n-n_t, \ldots, n \), which is not computationally feasible. Applying description length to neural networks in a meaningful and practical way therefore is highly non-trivial.

There are many methods for training neural networks. Our aim is not to develop new training methods, but rather to use description length for hyperparameter optimization with any training method. We would therefore like to find the description length for a neural network with a specific solution for the weights \( w \), fairly agnostically to how that solution was found. As mentioned, in the current paper we will limit ourselves to predictive MDL. In order to use predictive MDL, we need \( \hat{w}_i = \hat{\theta}_h(x', t') \) in step \( i \) of \( \text{(19)} \). For regression we need covariance estimates as well. Now to calculate \( \hat{\theta}_h(x', t') \) we could clearly use \( \hat{\theta}_h(x', t') \) as initialization, so that we do not need to do a full training at every stage. Therefore it could be quite computationally feasible to calculate the whole sequence \( \hat{\theta}_h(x^i, t^i), i = n-n_t, \ldots, n \). However, this raises several issues. One is that the sequence \( \hat{\theta}_h(x^i, t^i), i = n-n_t, \ldots, n \) might not converge to \( \hat{\theta}_h(x^n, t^n) \); by starting training on a small amount of data we might get an inferior solution, stuck in an undesirable local minimum; and as mentioned, our goal was to not change how we train the neural network, but check the outcome of a given training.
algorithm. Another issue is that updating $\hat{\theta}_h(x^i, t^i)$ with new data $(x_{i+1}, t_{i+1})$ is not a solved problem in neural network training.

The solution we propose is one we might call reverse unlearning. We start with $\hat{\theta}_h(x^n, t^n)$, which is obtained with any standard training algorithm. To find the solution $\hat{\theta}_h(x^{n-1}, t^{n-1})$ we use $\hat{\theta}_h(x^n, t^n)$ as initialization for training on $(x^{n-1}, t^{n-1})$; essentially we unlearn $(x_n, t_n)$. The idea is that the solution $\hat{\theta}_h(x^n, t^n)$ is at or near a local minimum of the cost function for $(x^n, t^n)$, as in [18], and that the cost function for $(x^{n-1}, t^{n-1})$ has a nearby local minimum. By retraining on $(x^{n-1}, t^{n-1})$ the initial solution $\hat{\theta}_h(x^n, t^n)$ moves to that local minimum—rather than jumping to another local minimum. We continue like that until we get a solution $\hat{\theta}_h(x^1, t^1)$. The idea is that the sequence of solutions $\hat{\theta}_h(t^i, x^i)$, $i = n - n_t, \ldots , n$ stays close to the original solution $\hat{\theta}_h(x^n, t^n)$, and the resulting description length therefore is a property of the specific solution $\hat{\theta}_h(x^n, t^n)$. The method is described in Alg. 1.

**Algorithm 1 Reverse Unlearning**

Train network on $(x^n, t^n)$ to obtain $\hat{\theta}_h(x^n, t^n)$, which are the weights $\hat{w}_n$ as well as covariance estimates for regression.

for $i = n - 1$ to $n - n_t$ do

Re-train the network on $(x^i, t^i)$ with $\hat{w}_{i+1}$ as initialization to obtain $\hat{\theta}_h(x^i, t^i)$.

Feed forward $x_{i+1}$ in the network with $\hat{\theta}_h(x^i, t^i)$ as parameters to obtain the distribution $P_{i+1}(\cdot)$.

end for

The code length is $C = \sum_{i=n-n_t+1}^{n} - \log P_{i}(t_i)$.
Figures 6-7 shows some experimental results. The setup is the same as for linear regression in Section 4. We train a single layer neural network with 15 hidden nodes on 75 random $x_n$ with observations $t_n = \sin(3x_n) + w_n$, where $w_n \sim \mathcal{N}(0,0.15)$. We seek to optimize the regularization parameter $\lambda$ in $L_2$ regularization. We use DDL with $n_t = \frac{3n}{4}$ and compare with cross-validation, where we use 25% of samples for cross-validation. Differential description length is aimed at minimizing log-loss, and Fig. 6 shows that it indeed performs better than cross-validation for log-loss. Fig. 7 shows the same results for mean square error (MSE). In this case, cross validation is set to minimize MSE, whereas DDL of course still aims at minimizing log-loss. Still, DDL outperforms cross-validation.

6 Conclusion

This paper has developed the framework for DDL. There is still much work to do to make this into a practical method. First, there are other methods for implementing DDL than predictive MDL. One is direct quantization of parameters, i.e., a literal implementation of (17). For reverse unlearning there are many theoretical and practical problems surrounding that goes to the depth of how neural networks learn. We also need to conduct experiments on larger, more realistic learning problems. Finally, the paper and methodology only develops a gauge for hyperparameter selection. To use this for large scale problems with many hyperparameters, optimization algorithms are needed such as those in Li et al. (2017), where it might be possible to use our gauge as an input to the optimization.
Figure 7: Single layer neural network (with 15 hidden nodes) trained on noisy sinusoidal data with $L_2$ regularization. The plot shows the distribution of MSE.

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