Machine Learning Course - CS-433

Model Selection and Cross-Validation

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Motivation

In ridge regression, the parameter $\lambda > 0$ can be tuned to reduce overfitting by reducing model complexity.

$$\min_{\mathbf{w}} \quad \frac{1}{2N}\sum_{n=1}^{N}[y_n - \widetilde{\boldsymbol{\phi}}(\mathbf{x}_n)^\top \mathbf{w}]^2 \quad + \quad \frac{\lambda}{2N}\sum_{j=0}^{M} w_j^2$$

But how do we choose λ? This is the *model selection* problem.

Probabilistic Setup

In order to answer the above question in a meaningful way we need to describe our mathematical framework. A fruitful and common such framework is probabilistic. We assume that there is an underlying distribution, call it $\mathcal{D}$, with range $\mathcal{Y} \times \mathcal{X}$. We do not know this distribution but we assume that the data set we see, call it S, consist of independent samples from $\mathcal{D}$:

$$S = \{(y_n, \mathbf{x}_n) \text{ iid} \sim \mathcal{D}\}_{n=1}^{N}.$$

Based on this sample the *learning algorithm* computes the "best" model within the class of given models. E.g., for ridge regression, with a fixed parameter λ, the learning algorithm computes the best weight function $\mathbf{w}$. We have seen that we can use e.g. (stochastic) gradient descent or least-squares for the ridge-regression model as an efficient way of implementing this learning. Let us write more generically $f_S = \mathcal{A}(S)$, where $\mathcal{A}$ denotes the learning algorithm, which depends on the sample S we are given and f_S is the "prediction function." E.g., in our previous example we have $f_S(\mathbf{x}) = \widetilde{\boldsymbol{\phi}}(\mathbf{x})^\top \mathbf{w}$, where $\mathbf{w}$ is the weight vector we computed. If we want to indicate that f_S also depends on parameters of the model, e.g., the λ in the ridge regression model, we can add a subscript to write $f_{S,\lambda}$.

Training Error versus Generalization Error

Given a prediction function f, how can we assess if f is any good? If we knew the distribution $\mathcal{D}$, then what we should do is to compute the *expected* error over all samples chosen according to $\mathcal{D}$, i.e., we should compute

$$L_{\mathcal{D}}(f) = \mathbb{E}_{\mathcal{D}}[\ell(y, f(\mathbf{x}))],$$

where $\ell(\cdot, \cdot)$ is our loss function. E.g., we have $\ell(y, f(\mathbf{x})) = (y - f(\mathbf{x}))^2$, i.e., the square loss, for the ridge regression problem.

This quantity has many names: *generalization error*, (true/-expected) risk, (true/expected) loss, to name just the most common ones. This is the quantity we are fundamentally interested in, but we cannot compute it since $\mathcal{D}$ is not known.

Since we do not know $\mathcal{D}$, but have given a sample S, it is natural to compute the equivalent *empirical* quantity

$$L_S(f) = \frac{1}{|S|} \sum_{(y_n, \mathbf{x}_n) \in S} \ell(y_n, f(\mathbf{x}_n)). \tag{1}$$

One of the problems with (1) is that in applications the prediction function f is *itself* a function of the data S. So in fact, by doing so, we compute the quantity

$$L_S(f_S) = \frac{1}{|S|} \sum_{(y,\mathbf{x}) \in S} \ell(y_n, f_S(\mathbf{x}_n)).$$

This is often called the *training error* and we have already discussed in previous lectures that this training error might not be representative of the error we see on "fresh" samples, i.e., $L_S(f_S)$ might not be close to $L_{\mathcal{D}}(f_S)$ due to overfitting.

Splitting the data

To avoid that we validate our model on the same sample we trained it on, it is natural that we split the data into a *training* and a *validation* set, e.g. 80% as training data and 20% as validation data, call them S_t and S_v, respectively. We apply the learning algorithm $\mathcal{A}$ to the training set S_t and compute the function f_{S_t}. We then compute the error on the validation set, i.e., we compute

$$L_{S_v}(f_{S_t}) = \frac{1}{|S_v|} \sum_{(y_n,\mathbf{x}_n) \in S_v} \ell(y_n, f_{S_t}(\mathbf{x}_n)).$$

Since S_v is a "fresh" sample we can hope that $L_{S_v}(f_{S_t})$ is close to the quantity $L_{\mathcal{D}}(f_{S_t})$. Indeed, in *expectation* both are the same, i.e.,

$$L_{\mathcal{D}}(f_{S_t}) = \mathbb{E}_{S_v \sim \mathcal{D}}[L_{S_v}(f_{S_t})], \tag{2}$$

where the expectation is over the samples of the validation set. But for a particular validation set S_v they might differ (e.g., there is fluctuation in $L_{S_v}(f_{S_t})$ due to the randomness of the validation set).

But we payed a price. We had to split the data and now have less data both for the learning as well as the validation task. A common trick to avoid this "loss of data" is to use "cross validation" techniques described at the end of this lecture. They seem to work well in practice but are hard to analyze.

Model selection

Recall that we are looking for a way to select (hyper)parameters of our model, like the parameter λ for the ridge regression problem. As we discussed, we split our data into a training set and validation set.

The set-up is hence the following. We have one training set S_t and one validation set S_v and we think of them as having been generated independently and sampled according to the underlying but unknown distribution $\mathcal{D}$. We have in addition a set of values for a parameter of the model, e.g., the parameter λ in the ridge regression problem. Let these values be λ_k, $k = 1, \cdots, K$. To keep things simple we assume that K is some finite value.

We run the learning algorithm K times on the same training set S_t to compute the K prediction functions f_{S_t,λ_k}. For each such prediction function we compute the empiricial risk/error/loss $L_{S_v}(f_{S_t,\lambda_k})$.

We then choose that value of the parameter λ which gives us the smallest such error.

In the figure below, we plot the empirical generalization error for many values of λ (grid search).

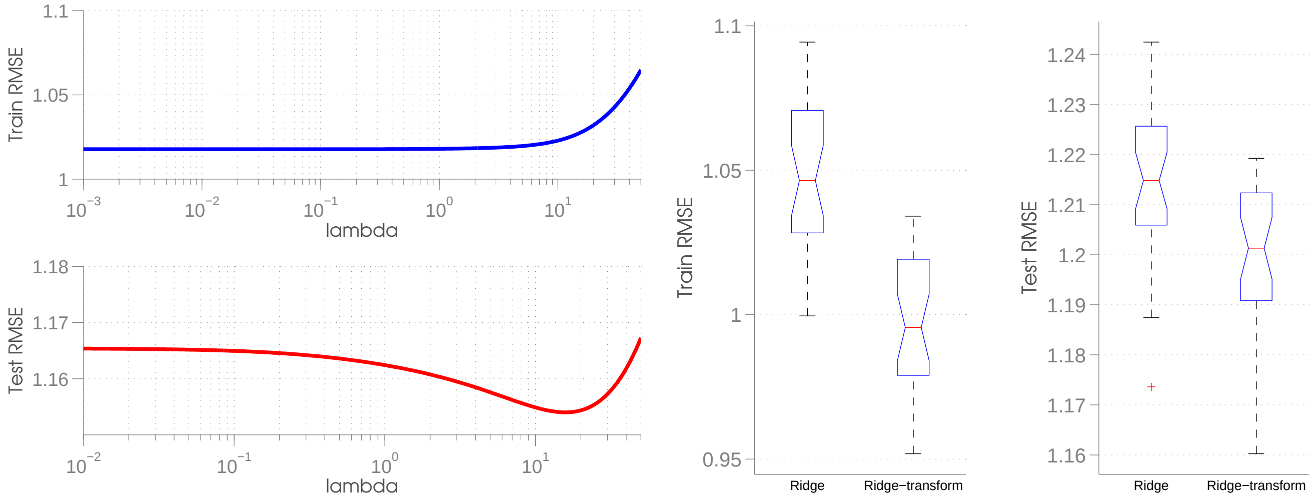


Figure 1: The left figure shows ridge regression results for a 50-50 split. The right one shows a comparison with and without feature transformations. The improvement is very little and might be insignificant.

Even if we use separate data sets for training and validation we still are faced with several questions. How do we know that the function $f_{S_t,\lambda}$ is a good approximation of the function $f_{\mathcal{D},\lambda}$, the best predictor within our class if we had access to the underlying distribution? We will discuss this issue in our next lecture. Similarly, how do we know that, for a fixed function f, $L_{S_v}(f)$ is a good approximation to $L_{\mathcal{D}}(f)$? Let us discuss this issue next.

True Error versus Empirical Error

Assume that we have K prediction functions f_k, $k = 1, \cdots, K$, and that our loss function $\ell(\cdot, \cdot)$ is bounded, lets say in $[0, 1]$. We are given a validation set S_v whose samples are chosen iid according to the underlying distribution $\mathcal{D}$. We compute the K empirical errors

$$L_{S_v}(f_k) = \frac{1}{|S_v|} \sum_{(y_n, \mathbf{x}_n) \in S_v} \ell(y_n, f_k(\mathbf{x}_n)).$$

Associated to these are the true errors

$$L_{\mathcal{D}}(f_k) = \mathbb{E}_{(y, \mathbf{x}) \sim \mathcal{D}}[\ell(y, f_k(\mathbf{x}))].$$

How far are these apart? We have seen in (2) that in expectation they are the same. So what we need to worry is the variation due to the finite size of the validation set. We claim that

$$\mathbb{P}\left\{ \max_k |L_{\mathcal{D}}(f_k)) - L_{S_v}(f_k)| \geq \sqrt{\frac{\ln(2K/\delta)}{2|S_v|}} \right\} \leq \delta. \quad (3)$$

This bound gives us some nice insights. First, the error goes down at least like one over the square root of the number of validation points we have. The more data points we have therefore, the more confident we can be that the empirical loss we measure is close to the true loss. Further, if we test K hyper-parameters our error only goes up by a very small amount which is proportional to $\sqrt{\ln(K)}$. So we can test quite a few different models without too much worry.

The proof of this statement is not very difficult. Since we assumed that each data sample $(y_n, \mathbf{x}_n)$ in the validation set S_v is chosen independently, the associated losses $\ell(y_n, \mathbf{x}_n)$ are also independent and identically distributed random variables, taking values in $[0, 1]$. Call each such loss Θ_n. The expected value of $\Theta_n = \ell(y_n, \mathbf{x}_n)$ is equal to the true loss

$L_{\mathcal{D}}(f)$ and we want to know the chance that the average of $|S_v|$ such idd values (this is the empirical loss $L_{S_v}(f)$) deviates from this expected value. This is exactly the set-up of the following lemma.

Lemma 0.1 (Chernoff Bound)**.** *Let $\Theta_1, \cdots, \Theta_N$ be a sequence of iid random variables with mean $\mathbb{E}[\Theta]$ and range $[0, 1]$. Then, for any $\epsilon > 0$,*

$$\mathbb{P}\{|\frac{1}{N}\sum_{n=1}^{N}\Theta_n - \mathbb{E}[\Theta]| \geq \epsilon\} \leq 2e^{-2N\epsilon^2}.$$

Using Lemma 0.1 let us show (3). Assume first that $K = 1$. Equating $2e^{-2|S_v|\epsilon^2}$ with δ we get that $\epsilon = \sqrt{\frac{\ln(2/\delta)}{2|S_v|}}$ as claimed.

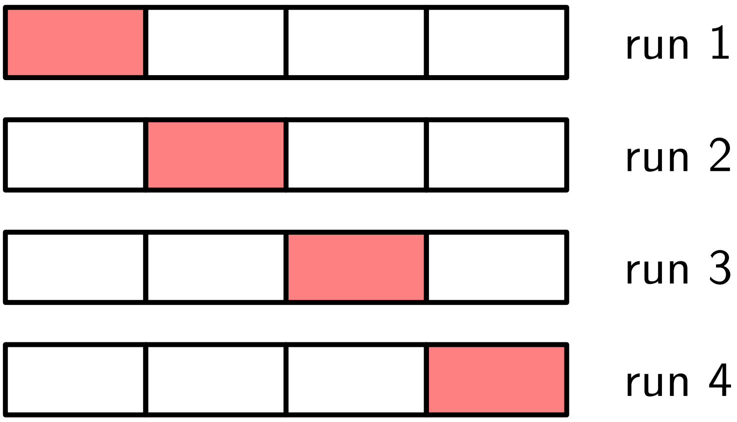
For a general K, if we check the deviations for K independent samples and ask for the probability that for at least one such sample we get a deviation of at least ϵ then by the union bound this probability is at most $2Ke^{-2|S_v|\epsilon^2}$. Hence, equating now $2Ke^{-2|S_v|\epsilon^2}$ with δ we get that $\epsilon = \sqrt{\frac{\ln(2K/\delta)}{2|S_v|}}$ as stated.

For completeness, we state at the very end of these notes a proof of Lemma 0.1.

Cross-validation

Random splits are not the most efficient way to compute the error.

K-fold cross-validation allows us to do this efficiently. We randomly partition the data into K groups. We train on $K-1$ groups and test on the remaining group. We repeat this until we have tested on all K sets. We then average the results.



Cross-validation returns an unbiased estimate of the *generalization error* and its variance.

Additional Notes

Proof of Lemma 0.1

Instead of considering the setup in the lemma we can equivalently assume that $\mathbb{E}[\Theta] = 0$ and that the Θ_n take values in $[a, b]$, where $a \leq 0 \leq b$ and $b - a = 1$. We will show that

$$\mathbb{P}\{\frac{1}{N}\sum_{n=1}^{N} \Theta_n xi \geq > \epsilon\} \leq e^{-2N\epsilon^2}.$$

This, together with the equivalent bound

$$\mathbb{P}\{\frac{1}{N}\sum_{n=1}^{N} \Theta_n \leq -\epsilon\} \leq e^{-2N\epsilon^2}$$

will prove the claim. We have

$$\begin{aligned}
\mathbb{P}\{\frac{1}{N}\sum_{n=1}^{N} \Theta_n \geq \epsilon\} &\overset{s>0}{=} \mathbb{P}\{e^{s\frac{1}{N}\sum_{n=1}^{N}\Theta_n} \geq e^{s\epsilon}\} \\
&\overset{(a)}{\leq} \min_{s>0}\mathbb{E}[e^{s\frac{1}{N}\sum_{n=1}^{N}\Theta_n}]e^{-s\epsilon} \\
&\overset{(b)}{=} \min_{s>0}\prod_{n=1}^{N}\mathbb{E}[e^{\frac{s\Theta_n}{N}}]e^{-s\epsilon} \\
&= \min_{s>0}\mathbb{E}[e^{\frac{s\Theta}{N}}]^N e^{-s\epsilon} \\
&\overset{(c)}{\leq} \min_{s>0}e^{s^2/(8N)}e^{-s\epsilon} \\
&\overset{s=4N\epsilon}{=} e^{-2N\epsilon^2}.
\end{aligned}$$

Here, step (a) follows from the Markov inequality. In step (b) we have used the fact that the random variables Θ_n, and hence the random variables $e^{\frac{s\Theta_n}{N}}$, are independent so that the expectation of the product is equal to the product of the expectations. Finally, in step (c) we have used the so-called Hoeffding lemma. It states that for any random variable X, with $\mathbb{E}[X] = 0$ and $X \in [a, b]$ we have

$$\mathbb{E}[e^{sX}] \leq e^{\frac{1}{8}s^2(b-a)^2}.$$

ToDo

- Implement CV and gain experience to set λ and K.
- Details on unbiasedness of cross-validation is in Section 7.10 in the book by Hastie, Tibshirani, and Friedman (HTF).
- Read about bootstrap in Section 7.11 in HTF book. This method is related to random splitting and is a very popular method.