STATS305A - Lecture 16

John Duchi
Scribed by Michael Howes

11/16/21

Contents

1 Announcements

- HW3 due Friday.
- Etude 3 due Friday and corrections due Monday.

Today we will be discussing two randomized methods - cross validation and permutation tests.

2 Validation

Suppose we have a fitting method $\widehat{\beta}$. We'd like to know how $\widehat{\beta}$ is going perform on future data. In a typical case we would have a hyperparameter λ and we want to pick the "best" λ. We have seen many examples of different things λ could represent, such as:

- We could have λ equal to the regularization parameter in ridge regression.
- We could also have λ equal to the number of coordinates in PC regression, forward stepwise regression or boosting.

Define

$$R(b) = \mathbb{E}[L(Y_{n+1}, X_{n+1}^T b)],$$

for some loss function $L : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$. The quantity $R(b)$ is the out-of-sample risk of the linear predictor $\widehat{y} = x^T b$. We wish to estimate $R(b)$ and choose λ which minimizes $R(\widehat{\beta})$. There are two approaches that we will discuss, using a hold out set or performing cross validation.

2.1 Hold out set

Hold out a subset of our data, call it the *validation data*. Fit the model on *training data* (which is all the data apart from the validation set). We can the calculate the average loss on the independent validation set. There are two issues with this

- It can be a little high variance.
- We are not using all the data.

2.2 Cross validation

The idea behind cross validation is to split our data into k equal sized partitions which we call *folds*. For each fold we fit on the remaining $k-1$ folds and then evaluate the model on the held out fold.

More mathematically, let $J(i)$ be the set of indices in fold i. Define

$$\widehat{\beta}^{-J(i)} = \text{model fit on } (X, Y) \text{ but with the indices in } J(i) \text{ removed.}$$

The emperical risk of using a linear predictor b on fold i is

$$\widehat{R}_i(b) = \frac{1}{|J(i)|} \sum_{i \in J(i)} L(y_j, x_j^T b),$$

where $|J(i)|$ is the cardinality of $J(i)$ which is typically $\frac{n}{k}$ (this happens when all the folds are the exact same size). Then define the k-fold cross validation error to be

$$CV(k) = \frac{1}{k} \sum_{i=1}^{k} \widehat{R}_i(\widehat{\beta}^{-J(i)}).$$

Two natural questions are:

(a) What is $CV(k)$ approximating?

(b) What do we use $CV(k)$ for?

Let $\mathcal{T}$ be a training set $(X, Y) \in \mathbb{R}^{n \times d} \times \mathbb{R}^n$. What we'd like to know is

$$\text{Err}(\mathcal{T}) = R(\widehat{\beta}(\mathcal{T})),$$

where $\widehat{\beta}(\mathcal{T})$ is the model trained using our test set $\mathcal{T}$. We'd like to know the expected error of using $\widehat{\beta}(\mathcal{T})$ on new data. Our training set is considered to be random and thus we can define

$$\text{Err}_n = \mathbb{E}[\text{Err}(\mathcal{T})],$$

where the expectation is taken over all training sets of size n. If we assume that our data is i.i.d. and the k folds all have size $\frac{n}{k}$, then

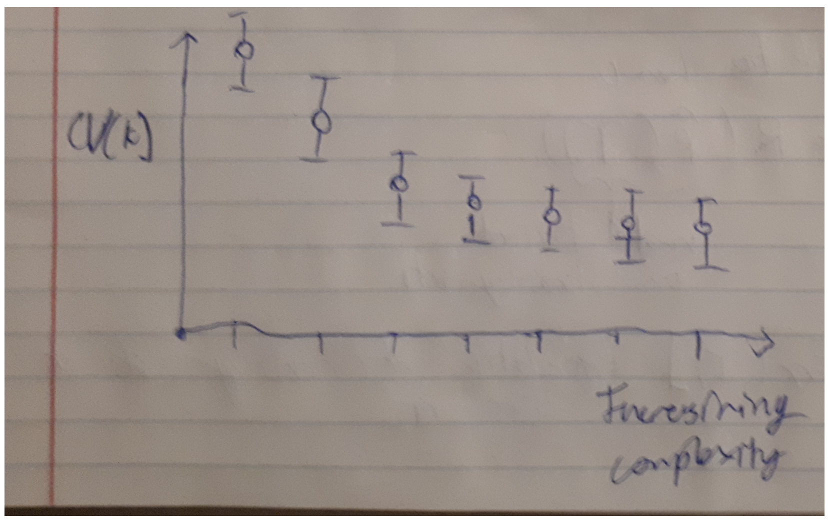
$$\begin{aligned}
\mathbb{E}[CV(k)] &= \mathbb{E}[\widehat{R}_k(\widehat{\beta}^{-J(k)})] \\
&= \mathbb{E}\left[\mathbb{E}\left[\widehat{R}_k(\widehat{\beta}^{-J(k)})\middle| -J(k)\right]\right] \\
&= \mathbb{E}[R(\widehat{\beta}(\text{training set of size } n - k/n))] \\
&= \text{Err}_{\frac{(k-1)n}{k}} +
\end{aligned}$$

Thus we have an issue $\mathbb{E}[CV(k)]$ is not unbiased for Err_n. There are some "solutions"

- Just ignore the bias.
- Introduce correction terms. These can be a bit complicated and will depend on the loss function L and the choice of model fitting procedure. See John's notes for some details in special cases.
- If we take k large, $\text{Err}_{\frac{(k-1)n}{k}}$ will be close to n. We will discuss this more in the leave one out section.

2.3 Using cross validation for model selection

In partice we calculate $CV(k)$ for various values of λ and then compare $CV(k)$ accross these values. If we plot $CV(k)$ we tend to see pictures that look like this:



As we increase complexity (ie increase $\frac{1}{\lambda}$ in ridge regression or increase the number of components in PCA regression/forward stepwise), $CV(k)$ decreases. We can put error bars on $CV(k)$ by calculating the emperical standard deviation of $CV(k)$. This gives us the error bars in the plot. One may to choose λ^* is to take the least complex model for which all the "more complex" models have $CV(k)$ within one standard error. We then fit a model using the full data and this chosen value of λ^*.

2.4 Leave one out cross validation

Returning to the idea of taking k large, we can set $k = n$. This is nice because then $CV(k)$ is unbiased for $\text{Err}_{\frac{n-1}{n}}$ which should be close to Err_n. When $k = n$ each fold is a single data point and so we set $J(i) = \{i\}$. There are two issues:

- This may by computationally challenging we have to fit n models for each model fitting procedure.
- The variance of $CV(n)$ may be larger than when $k = 5$ or $k = 10$ (this is still disputed).

In ordinary least squares we have computational tricks that means that n-fold cross validation can be done quickly. Suppose that we are using the model $y = X\beta + \varepsilon$ to fit $\widehat{\beta}$. That is $\widehat{\beta} = (X^TX)^{-1}X^Ty$ and

$$\widehat{y} = X\widehat{\beta} = X(X^TX)^{-1}X^Ty = Hy.$$

If we let H_{ii} be the leverage scores of the model (the diagonal entries of H), then we have previously seen that

$$\widehat{y}_i = H_{ii}y + (1 - H_{ii})\widehat{y}_{-i},$$

where $\widehat{y}_{-i} = x_i^T \widehat{\beta}^{-i}$ is the prediction for y_i given only (X_{-i}, y_{-i}). Thus we have

$$\widehat{y}_{-i} = \frac{y_i}{1 - H_{ii}} \widehat{y}_i - \frac{H_{ii}}{1 - H_{ii}} y_i.$$

And so

$$y_i - \widehat{y}_{-i} = \frac{y_i - \widehat{y}_i}{1 - H_i i}.$$

Thus for fitting $\widehat{\beta} = (X^T X)^{-1} X$ we have

$$CV(n) = \frac{1}{n} \sum_{i=1}^{n} \frac{(y_i - \widehat{y}_i)^2}{(1 - H_{ii})^2},$$

under square error loss. This method can be used when λ determines X and then $\widehat{\beta}$ is given by ordinary least square regression.

In general, computing $\widehat{\beta}^{-i}$ can sometimes be easy and sometimes very hard. Suppose that instead of squared error we fit a model with the more general loss

$$L_n(b) = \frac{1}{n} \sum_{i=1}^{n} l(y_i - x_i^T b).$$

A very effective stratergy is to approximate L_n with a quadratic at $\widehat{\beta} = \operatorname{argmin}_b L_n(b)$, then remove the i^{th} term and choose $\widehat{\beta}^{-i}_{\text{quad}}$ to be the value which minimizes the approximation. More specifically we have

$$L_n(b) \approx L_n(\widehat{\beta}) - \frac{1}{n} \sum_{i=1}^{n} l'(y_i - x_i^T \widehat{\beta}_i) x_i^T (b - \widehat{\beta}) + \frac{1}{2n} \sum_{i=1}^{n} (b - \widehat{\beta})^T l''(y_i - x_i^T \widehat{\beta}) x_i x_i^T (b - \widehat{\beta}).$$

Define $\widehat{\varepsilon}_i = y_i - x_i^T \widehat{\beta}$, then

$$\begin{aligned}
L_{-i}(b) &= \frac{1}{n-1} \sum_{j \neq i} L_j(y_j - x_j^T b) \\
&\approx \frac{1}{n-1} \sum_{j \neq i} L_j(\widehat{\varepsilon}_j) - \frac{1}{n-1} \sum_{j \neq i} l'(\widehat{\varepsilon}_j) x_i^T (b - \widehat{\beta}) + \frac{1}{2(n-1)} \sum_{j \neq i} (b - \widehat{\beta})^T l''(\widehat{\varepsilon}_j) x_i x_i^T (b - \widehat{\beta}) \\
&= c + g_{-i}^T b + \frac{1}{2} b^T A_{-i} b,
\end{aligned}$$

where

$$g_{-i} = -\frac{1}{n-1} \sum_{j \neq i} \left(l'(\widehat{\varepsilon}_j) x_j + l''(\widehat{\varepsilon}_j) x_j x_j^T \widehat{\beta} \right),$$

and

$$A_{-i} = \frac{1}{n-1} \sum_{j \neq i} l''(\widehat{\varepsilon}_j) x_j x_j^T.$$

The minimizer of the quadratic approximation is

$$\widehat{\beta}^{-i}_{\text{quad}} = -A_{-i}^{-1} g_{-i}.$$

Note that the matrix A_{-i} differs from the Hessian of $L_n(\widehat{\beta})$ by a rank one update. Thus inverting A_{-i} can be done quickly provided that we have stored the inverse Hessian.

3 Permuation testing

We will leverage the fact that if two random variables have no relationship (ie X_i and Y_i are independent), then

$$(X_i, Y_i)_{i=1}^n \overset{\text{dist}}{=} (X_i, Y_{\pi(i)})_{i=1}^n,$$

where $\pi : [n] \to [n]$ is a permutation of $[n] = \{1, 2, \ldots, n\}$. Thus under independence, any statistic $T_n = T((X_i, Y_i)_{i=1}^n)$ should have the same distribution under permutations i.e.

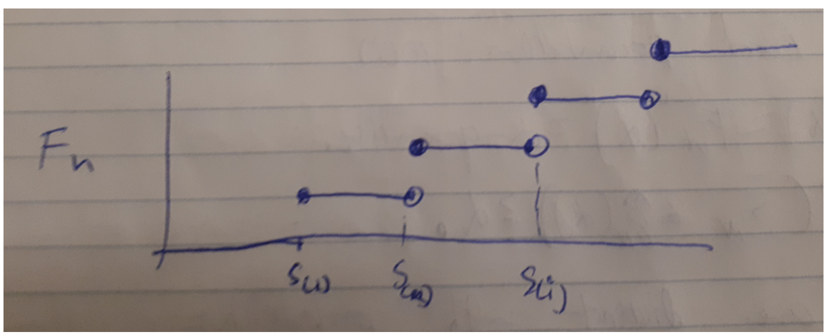
$$T_n \overset{\text{dist}}{=} T((X_i, Y_{\pi(i)})_{i=1}^n).$$

Definition 1. Let $S_1, \ldots, S_N$ be real values statistics and define the *emprical CDF* of s_i to be

$$F_N(t) = \frac{1}{N} \sum_{i=1}^{N} \mathbb{I}(S_i \leq t),$$

where $\mathbb{I}(S_i \leq t)$ is 1 if $S_i \leq t$ and 0 otherwise.

The function F_N is a step function that looks something like this:

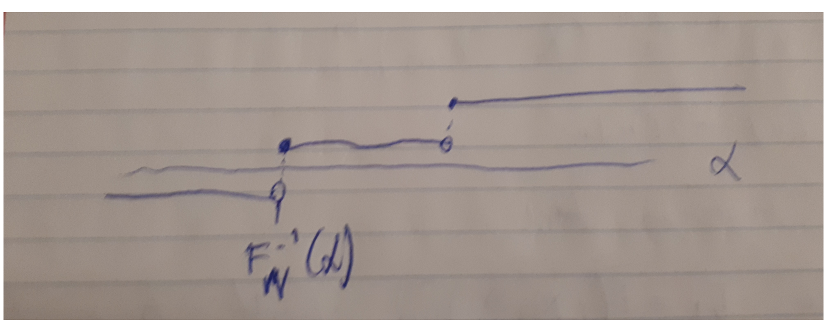


Note that $F_N(t)$ is right continuous.

Definition 2. With S_i as before define the *quartile function* to be

$$\widehat{q}_N(\alpha) = F_N^{-1}(\alpha) = \inf\{t \in \mathbb{R} : F_N(t) \geq \alpha\}.$$

The qunatile function looks like this:



Note that $F_N(F_N^{-1}(\alpha)) \geq \alpha$ for all α and that $F_N^{-1}(i/N) = S_{(i)}$ if

$$S_{(1)} < S_{(2)} < \ldots < S_{(N)}.$$

Theorem 1. *Suppose that the statistics $S_1, \ldots, S_N$ are exchangable and so that for all permutations π*

$$(S_1, \ldots, S_N) \stackrel{dist}{=} (S_{\pi(1)}, \ldots S_{\pi(N)}).$$

Let $\widehat{q}_N = F_N^{-1}$ be the quartile function. Then

$$\mathbb{P}(S_N \le \widehat{q}_N(\alpha)) \ge \alpha,$$

for all α. If $S_1, \ldots, S_N$ are all distinct with probability one, then

$$\mathbb{P}(S_N \le \widehat{q}_N(\alpha)) \le \alpha + \frac{1}{N}.$$

Proof. Note that for all i, $\mathbb{P}(s_i \le \widehat{q}_N(\alpha)) = \mathbb{P}(S_N \le \widehat{q}_N(\alpha))$ by exchangability. Thus

$$\begin{aligned}\mathbb{E}[F_N(\widehat{q}_N(\alpha))] &= \frac{1}{N}\sum_{i=1}^{N} \mathbb{P}(S_i \le \widehat{q}_N(\alpha)) \\ &= \mathbb{P}(S_N \le \widehat{q}_N(\alpha)).\end{aligned}$$

We also know that $F_N(\widehat{q}_N(\alpha)) \ge \alpha$ and so

$$\mathbb{P}(S_N \le \widehat{q}_N(\alpha)) = \mathbb{E}[F_N(\widehat{q}_N(\alpha))] \ge \alpha.$$

And if S_i are distinct then the size of the jumps in F_N are exactly $\frac{1}{N}$ and so

$$F_N(\widehat{q}_N(\alpha)) \le \alpha + \frac{1}{N}.$$

This thus implies

$$\mathbb{P}(S_N \le \widehat{q}_N(\alpha)) = \mathbb{E}[F_N(\widehat{q}_N(\alpha))] \le \alpha + \frac{1}{N}.$$

□

The upshot is that we should think of $\mathbb{P}(S_N \le \widehat{q}_N(\alpha))$ as being equal to α but there is some error due to discretization. The error has size $\le \frac{1}{N}$.

Note that as a consequence we have $\mathbb{P}(S_N > \widehat{q}_N(\alpha)) \le \alpha$ since

$$\mathbb{P}(S_N > \widehat{q}_N(\alpha)) = 1 - \mathbb{P}(S_N \le \widehat{q}_N(\alpha)) \le 1 - (1 - \alpha) = \alpha.$$

Example 1. Say we have i.i.d data (X_i, Y_i) and we want to test the null $H_0 : X_i \perp\!\!\!\perp Y_i$. Under the null, $(X_i, Y_i) \stackrel{\text{dist}}{=} (X_i, Y_{\pi(i)})$. We can fit $\widehat{\beta} = (X^T X)^{-1} X^T Y$ and $\widehat{\beta}_\pi = (X^T X)^{-1} X^T Y_\pi$ where

$$Y_\pi = \begin{bmatrix} Y_{\pi(1)} \\ \vdots \\ Y_{\pi(n)} \end{bmatrix}.$$

Suppose we do this for $m-1$ random permuations. Set $S_m = \left\|\widehat{\beta}\right\|_2^2$ (although we could use <u>any</u> function of $\widehat{\beta}$) and $S_i = \left\|\widehat{\beta}_\pi\right\|_2^2$. We can then reject H_0 if

$$S_m \ge \text{ Quantile}_{1-\alpha}(S_{\pi_i}, S_m).$$

This test will have level α.