Almost-Cross-Validation Theorem

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We are interested in bounding the error of the selected model when tuning penalty parameters by a "modified averaged version of cross-validation". Our result is an application of Mitchell's result to penalized regression problems where the fitted functions are smooth with respect to the penalty parameters.

Suppose that the data is generated from the model

$$y = g^*(x) + \epsilon$$

Suppose the errors are independent and bounded ($\|\epsilon\|_\infty < \infty$).

The penalized regression model fitted on dataset D is denoted

$$\hat{g}_D(\cdot|\boldsymbol{\lambda}) = \arg\min_{g \in \mathcal{G}} L_D(g|\boldsymbol{\lambda})$$

Split data D into K folds, where each fold is D_k and $D_{-k} = D \backslash D_k$. Suppose D has size n, D_k all have size n_V, and D_{-k} all have size n_T.

We select penalty parameters such that

$$\hat{\boldsymbol{\lambda}} = \arg\min_{\lambda} \sum_{k=1}^K \|y - \hat{g}_{D_{-k}}(\cdot|\boldsymbol{\lambda})\|_k^2$$

We consider the behavior of the "modified averaged version of cross-validation"

$$\hat{g}_{MCV}(\cdot|D) = \frac{1}{K}\sum_{k=1}^K \hat{g}_{D_{-k}}(\cdot|\boldsymbol{\lambda})$$

Under sufficient entropy conditions, the error of the selected model will converge to the error of the oracle.

We are interested in bounding its generalization error

$$E_D\|\hat{g}_{MCV}(\cdot|D) - g^*\|^2 = E_D\left[\int \left(\hat{g}_{MCV}(x|D) - g^*(x)\right)^2 d\mu(x)\right]$$

1 Theorem 2

We will assume that $\sup_{g \in \mathcal{G}} \|g\|_\infty \leq G$.

Suppose that for all $k = 1, ..., K$, the following smoothness condition holds:

$$\|\hat{g}_{D_{-k}}(\cdot|\boldsymbol{\lambda}_1) - \hat{g}_{D_{-k}}(\cdot|\boldsymbol{\lambda}_2)\|_\infty \leq C n^\kappa \|\boldsymbol{\lambda}_1 - \boldsymbol{\lambda}_2\|$$

Then for all $a > 0$,

$$E\left[\|g^* - \hat{g}_{MCV}(\cdot|D)\|^2\right] \leq (1+a) \min_{\lambda \in \Lambda} E_{D^{(n_T)}}\left[\|g^* - \hat{g}_{D^{(n_T)}}(\cdot|\boldsymbol{\lambda})\|^2\right] + \frac{c_a}{n_V}\left[c_1 \log n_T + c_2 J \log n_V + c_3\right]$$

where c_1, c_2, c_3, c_a are constants.

Proof

We apply Theorem 3.5 in Mitchell's paper. We consider the loss function $Q(x, g) = (g(x) - g^*(x))^2$. Clearly $Q(x, g^*) = 0$. We will use the set of statistics

$$\mathcal{G}(T) = \{\hat{g}_T(\cdot|\boldsymbol{\lambda})\}$$

where T is some training data.

1. Establish Assumptions A.1 and A.2 are satisfied:

Theorem 3.5 relies on assumption A.1 and A.2 to be satisfied.

Assumption A.1 states that the Orlicz norm with $\psi_1 = \exp(x) - 1$ is bounded for some constant K_0:

$$\left\|(\hat{g}_D(\cdot|\boldsymbol{\lambda}) - g^*)^2\right\|_{L_{\psi_1}} \leq K_0$$

where

$$\|f\|_{\psi_1} = \inf\{C > 0 : E\psi(|f|/C) \leq 1\}$$

Since we have assumed that $\|g\|_\infty \leq G$, then by Lemma Orlicz-norm-properties (see Appendix)

$$\left\|(\hat{g}_D(\cdot|\boldsymbol{\lambda}) - g^*)^2\right\|_{L_{\psi_1}} \leq 2\left\|(\hat{g}_D(\cdot|\boldsymbol{\lambda}) - g^*)^2\right\|_\infty \leq 8G^2$$

Assumption A.2 states that

$$\left\|(\hat{g}_D(\cdot|\boldsymbol{\lambda}) - g^*)^2\right\|_{L_2} \leq K_1 \|\hat{g}_D(\cdot|\boldsymbol{\lambda}) - g^*\|_{L_2}$$

To see that this is satisfied, note that

$$\begin{aligned}
\left\|(\hat{g}_D(\cdot|\boldsymbol{\lambda}) - g^*)^2\right\|_{L_2}^2 &= \int (g^*(x) - \hat{g}_D(\cdot|\boldsymbol{\lambda}))^4 \, d\mu(x) \\
&\leq \left\|(g^* - \hat{g}_D(\cdot|\boldsymbol{\lambda}))^2\right\|_{L_1} \left\|(g^* - \hat{g}_D(\cdot|\boldsymbol{\lambda}))^2\right\|_{\infty} \\
&\leq 4G^2 \left\|g^* - \hat{g}_D(\cdot|\boldsymbol{\lambda})\right\|_{L_2}^2
\end{aligned}$$

2. Calculate the L_2 and ψ_1 entropies

Theorem 3.5 requires calculating the entropies of the excess loss functions

$$\mathcal{Q}(T) = \left\{ Q(x|\boldsymbol{\lambda}) = (\hat{g}_T(x|\boldsymbol{\lambda}) - g^*(x))^2 : \lambda \in \Lambda \right\}$$

where T is any training dataset.

We are interested in calculating the $\|\cdot\|_{\psi_1}$ and $\|\cdot\|_{L_2}$ entropy of the function class

$$\mathcal{Q}_d^{L_2}(T) = \left\{ Q \in \mathcal{Q}(T) : \|Q\|_{L_2} \leq \sqrt{d} \right\}$$

To bound these two entropies, we'll actually bound $H(u, \mathcal{Q}_d^{L_2}(T), \|\cdot\|_\infty)$ since

$$H(u, \mathcal{Q}_d^{L_2}(T), \|\cdot\|_{\psi_1}) \leq H(u/2, \mathcal{Q}_d^{L_2}(T), \|\cdot\|_\infty)$$

and

$$H(u, \mathcal{Q}_d^{L_2}(T), \|\cdot\|_{L_2}) \leq H(u, \mathcal{Q}_d^{L_2}(T), \|\cdot\|_\infty)$$

We show that the excess log functions $Q(x|\boldsymbol{\lambda})$ are smoothly parametric in $\boldsymbol{\lambda}$:

$$\begin{aligned}
\|Q(x|\boldsymbol{\lambda}_1) - Q(x|\boldsymbol{\lambda}_2)\|_\infty &= \left\|(\hat{g}_T(x|\boldsymbol{\lambda}_1) - g^*(x))^2 - (\hat{g}_T(x|\boldsymbol{\lambda}_2) - g^*(x))^2\right\|_\infty \\
&= \|(\hat{g}_T(x|\boldsymbol{\lambda}_1) - \hat{g}_T(x|\boldsymbol{\lambda}_2))\,(\hat{g}_T(x|\boldsymbol{\lambda}_1) + \hat{g}_T(x|\boldsymbol{\lambda}_2) - 2g^*(x))\|_\infty \\
&\leq \|\hat{g}_T(x|\boldsymbol{\lambda}_1) - \hat{g}_T(x|\boldsymbol{\lambda}_2)\|_\infty \|\hat{g}_T(x|\boldsymbol{\lambda}_1) + \hat{g}_T(x|\boldsymbol{\lambda}_2) - 2g^*(x)\|_\infty
\end{aligned}$$

Under the assumption that

$$\|\hat{g}_T(x|\boldsymbol{\lambda}_1) - \hat{g}_T(x|\boldsymbol{\lambda}_2)\|_\infty \leq Cn^\kappa \|\boldsymbol{\lambda}_1 - \boldsymbol{\lambda}_2\|$$

then

$$\|Q(x|\boldsymbol{\lambda}_1) - Q(x|\boldsymbol{\lambda}_2)\|_\infty \leq 4GCn^\kappa \|\boldsymbol{\lambda}_1 - \boldsymbol{\lambda}_2\|$$

Hence

$$
\begin{aligned}
H(u, \mathcal{Q}_d^{L_2}(T), \|\cdot\|_\infty) &\leq H\left(\frac{u}{4GCn^\kappa}, \Lambda, \|\cdot\|_2\right) \\
&\leq \log\left[\frac{1}{C_J}\left(\frac{16GCn^\kappa\lambda_{max} + 2u}{u}\right)^J\right]
\end{aligned}
$$

Hence

$$
H(u, \mathcal{Q}_d^{L_2}(T), \|\cdot\|_{\psi_1}) \leq \log\left[\frac{1}{C_J}\left(\frac{32GCn^\kappa\lambda_{max} + 2u}{u}\right)^J\right]
$$

and

$$
H(u, \mathcal{Q}_d^{L_2}(T), \|\cdot\|_{L_2}) \leq \log\left[\frac{1}{C_J}\left(\frac{16GCn^\kappa\lambda_{max} + 2u}{u}\right)^J\right]
$$

We calculate each component of the complexity term $J(d)$:

$$
\begin{aligned}
\gamma_1(\mathcal{Q}_d^{L_2}(T), \|\cdot\|_{\psi_1}) &\leq \int_0^{2G} H(u, \mathcal{Q}_d^{L_2}(T), \|\cdot\|_{\psi_1}) du \\
&= \int_0^{2G} \log\left[\frac{1}{C_J}\left(\frac{32GCn^\kappa\lambda_{max} + 2u}{u}\right)^J\right] du \\
&= 2G\int_0^1 \log\left(\frac{1}{C_J}\right) + J\log\left(\frac{32GCn^\kappa\lambda_{max} + 4Gv}{2Gv}\right) dv \\
&\leq 2G\left[\int_0^1 \log\left(\frac{1}{C_J}\right) + J\log\left(\frac{32Cn^\kappa\lambda_{max}}{v}\right) + J\log 4 dv\right] \\
&\leq 2G\left[\log\left(\frac{1}{C_J}\right) + J\left(1 + \log 4 + \log\left(32Cn^\kappa\lambda_{max}\right)\right)\right]
\end{aligned}
$$

and

$$\begin{aligned}
\gamma_2(\mathcal{Q}_d^{L_2}(T), \|\cdot\|_{L_2}) &= \int_0^{\sqrt{d}} \left[H(u, \mathcal{Q}_d^{L_2}(T), \|\cdot\|_{L_2})\right]^{1/2} du \\
&= \sqrt{d}\int_0^1 \left(\log\left[\frac{1}{C_J}\left(\frac{16GCn^\kappa\lambda_{max} + 2\sqrt{d}v}{\sqrt{d}v}\right)^J\right]\right)^{1/2} dv \\
&\leq \sqrt{d}\left[\int_0^1 \log\left(\frac{1}{C_J}\right) + J\log\left(\frac{32GCn^\kappa\lambda_{max}}{\sqrt{d}}\right) + J\log\frac{1}{u} + J\log 4du\right]^{1/2} \\
&= \sqrt{d}\left[\log\left(\frac{1}{C_J}\right) + J\left(1 + \log 4 + \log\left(\frac{32GCn^\kappa\lambda_{max}}{\sqrt{d}}\right)\right)\right]^{1/2}
\end{aligned}$$

3. Apply Theorem 3.5

Now we must select an increasing function J such that J^{-1} is strictly convex and

$$J(d) \geq \gamma_2(\mathcal{Q}_d^{L_2}(T), \|\cdot\|_{L_2}) + \frac{(\log n_T)\,\gamma_1(\mathcal{Q}_d^{L_2}(T), \|\cdot\|_{\psi_1})}{\sqrt{n_V}} \forall d \geq d_{min}$$

Let us choose $d_{min} = 1/n_V$. Then note that

$$\gamma_2(\mathcal{Q}_d^{L_2}(T), \|\cdot\|_{L_2}) \leq \sqrt{d}\left[\log\left(\frac{1}{C_J}\right) + J\left(1 + \log 4 + \log\left(32GCn^\kappa\sqrt{n_V}\lambda_{max}\right)\right)\right]^{1/2}$$

Then let

$$K_{n,1} = \left[\log\left(\frac{1}{C_J}\right) + J\left(1 + \log 4 + \log\left(32GCn^\kappa\sqrt{n_V}\lambda_{max}\right)\right)\right]^{1/2}$$

and

$$K_{n,2} = \frac{(\log n_T)\,2G\left[\log\left(\frac{1}{C_J}\right) + J\left(1 + \log 4 + \log\left(32Cn^\kappa\lambda_{max}\right)\right)\right]}{\sqrt{n_V}}$$

We define

$$J(d) \coloneqq \sqrt{d}K_{n,1} + K_{n,2}$$

Then$J^{-1}(b)$ is

$$J^{-1}(b) = \left(\frac{b - K_{n,2}}{K_{n,1}}\right)^2$$

The convex conjugate of $J^{-1}(b)$ is

$$
\begin{aligned}
\psi(z) &= \sup_x xz - J^{-1}(x) \\
&= \sup_x xz - \left(\frac{x - K_{n,2}}{K_{n,1}}\right)^2 \\
&= \frac{K_{n,1}^2 z^2}{4} + K_{n,2} z
\end{aligned}
$$

Note that $\psi(z)/z^r$ is a decreasing function in z for all $r > 2$. Also $\lim_{z\to\infty} \psi(z) = \infty$.
Theorem 3.5 states that for all $a > 0, q > 1$, we have

$$
E\left[\|g^* - \hat{g}_{MCV}(\cdot|D)\|^2\right] \le (1+a) \min_{\lambda\in\Lambda} E_{D^{(n_T)}}\left[\|g^* - \hat{g}_{D^{(n_T)}}(\cdot|\boldsymbol{\lambda})\|^2\right] + \frac{ac\epsilon_q(1/q)}{q}
$$

where $\epsilon_q(u) = \psi\left(\frac{2q^{r+1}(1+a)u}{a\sqrt{n_V}}\right) \vee \frac{1}{n_V} \forall u > 0$.
To calculate $\epsilon_q(1/q)$ (with $r = 3$), note that

$$
\psi\left(\frac{2q^4(1+a)\frac{1}{q}}{a\sqrt{n_V}}\right) = \frac{K_{n,1}^2}{4}\left(\frac{2q^3(1+a)}{a\sqrt{n_V}}\right)^2 + K_{n,2}\left(\frac{2q^3(1+a)}{a\sqrt{n_V}}\right)
$$

Finally, we get

$$
E\left[\|g^* - \frac{1}{k}\sum_{k=1}^{K} g_{\hat{\lambda}}(\cdot|D_{-k})\|^2\right] \le (1+a)E\left[\|g^* - \frac{1}{k}\sum_{k=1}^{K} g_{\tilde{\lambda}}(\cdot|D_{-k})\|^2\right] + ac\left(\frac{K_{n,1}^2}{4}q^5\left(\frac{2(1+a)}{a\sqrt{n_V}}\right)^2 + K_{n,2}\left(\frac{2q^2(1+a)}{a\sqrt{n_V}}\right)\right)
$$

where

$$
K_{n,1} = \left[\log\left(\frac{1}{C_J}\right) + J\left(1 + \log 4 + \log\left(32GCn^\kappa\sqrt{n_V}\lambda_{max}\right)\right)\right]^{1/2}
$$

and

$$
K_{n,2} = \frac{(\log n_T)\, 2G\left[\log\left(\frac{1}{C_J}\right) + J\left(1 + \log 4 + \log\left(32Cn^\kappa\lambda_{max}\right)\right)\right]}{\sqrt{n_V}}
$$

The last term is $1/n_V$. We can just swap out constants to see this:

$$
E\left[\|g^* - \hat{g}_{MCV}(\cdot|D)\|^2\right] \le (1+a)\min_{\lambda\in\Lambda} E_{D^{(n_T)}}\left[\|g^* - \hat{g}_{D^{(n_T)}}(\cdot|\boldsymbol{\lambda})\|^2\right] + \frac{ac}{n_V}\left(\frac{K_{n,1}^2}{4}q^5\left(\frac{2(1+a)}{a}\right)^2 + C_{n,2}\left(\frac{2q^2(1+a)}{a}\right)\right)
$$

where $C_{n,2}$ is the numerator of $K_{n,2}$.

2 Appendix

2.0.1 Lemma: Orlicz Norm Properties

For any function f, we have

$$\|f\|_{\psi_1} \leq 2\|f\|_\infty$$

Also

$$\|Kf\|_\psi = K\|f\|_\psi$$

Also suppose that ψ is a monotone function. Then

$$\|gf\|_\psi \leq \|g\|_\infty \|f\|_\psi$$

Proof

To prove the bound:

$$E\left[\exp\left(\frac{f}{2\|f\|_\infty}\right) - 1\right] \leq \exp\frac{1}{2} - 1 < 1$$

To prove the norm scaling property:

$$\begin{aligned}
\|Kf\|_\psi &= \inf\{C > 0 : E\psi(|Kf|/C) \leq 1\} \\
&= \inf\{C > 0 : E\psi(|f|/(C/K)) \leq 1\} \\
&= \inf\{KC > 0 : E\psi(|f|/C) \leq 1\} \\
&= K \inf\{C > 0 : E\psi(|f|/C) \leq 1\} \\
&= K\|f\|_\psi
\end{aligned}$$

To prove the last bound, note that under the assumption that ψ is a monotone function, then

$$E\psi(|gf|/C) \leq E\psi\left(|\|g\|_\infty f|/C\right)$$

Therefore

$$\inf_C E\psi(|gf|/C) \leq \inf_C E\psi\left(|\|g\|_\infty f|/C\right)$$

Therefore

$$\begin{aligned}
\|gf\|_\psi &= \inf\{C > 0 : E\psi(|gf|/C) \leq 1\} \\
&\leq \inf\{C > 0 : E\psi\left(|\|g\|_\infty f|/C\right) \leq 1\} \\
&= \|g\|_\infty \inf\{C > 0 : E\psi\left(|f|/C\right) \leq 1\} \\
&= \|g\|_\infty \|f\|_\psi
\end{aligned}$$