Oracle Inequalities for multiple penalty parameters

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Abstract

In penalized regression problems, the choice of penalty parameters is important since they ultimately determine the fitted model. The penalty parameters that minimize the generalization error are generally unknown and must be estimated. In this paper, we establish finite-sample oracle inequalities for models selected by a validation set approach. Our upper bounds on the model error depend on the oracle error and a near-parametric term. Therefore in settings where the oracle error shrinks at a sub-parametric rate, the number of penalty parameters can grow with the sample size without affecting the asymptotic convergence rate. Our oracle inequalities hold for penalized regression problems where the fitted models are smoothly parameterized by the penalty parameters. We show that this smoothness condition is satisfied by adding a ridge penalty to the training criterion.

Keywords: Regression, Cross-validation, Regularization

1 Introduction

Per the usual regression framework, we observe response $y \in \mathbb{R}$ and predictors $\boldsymbol{x} \in \mathbb{R}^p$. Suppose y is generated from the model g^* from model class $\mathcal{G}$

$$y = g^*(\boldsymbol{x}) + \epsilon \tag{1}$$

where ϵ_i are random errors with expectation zero. Our goal is to find the best model in $\mathcal{G}$ to model y given $\boldsymbol{x}$.

In high-dimensional $(p \gg n)$ or ill-posed problems, the ordinary least squares estimate performs poorly as it overfits to the training data. A common solution is to add regularization, or penalization, to control model complexity and induce desired structure. The penalized least squares estimate minimizes a criterion of the form

$$\hat{g}(\cdot|\boldsymbol{\lambda}) = \arg\min_{g \in \mathcal{G}} \frac{1}{n} \sum_{i=1}^{n} (y_i - g(x_i))^2 + \sum_{j=1}^{J} \lambda_j P_j(g) \tag{2}$$

where P_j are the penalty functions and λ_j are the penalty parameters.

Selecting the penalty parameters is an important task since they ultimately determine the fitted model. Their oracle values balance the residual least squares and the penalty terms to ensure fast convergence rates (van de Geer 2000). For example, when fitting an additive model $f(\boldsymbol{x}) = \sum_{j=1}^{J} f_j(x_j)$ with a roughness penalty for each component, the penalty parameters should be inversely proportional to the penalties of the true model (van de Geer & Muro 2014). When fitting a linear model using the lasso, the penalty parameter should be on the order $\sigma(\log p/n)^{1/2}$ where σ^2 is the variance of the error terms (Bühlmann & Van De Geer 2011).

The obvious problem is that the oracle penalty parameters depend on unknown values. Thus penalty parameters are usually tuned via a training/validation split or cross-validation. The basic idea is to train a model on a random partition of the data and evaluate its error on the remaining data. The penalty parameters that minimize the error on this validation set are then selected. For a more complete review of cross-validation, refer to Arlot (Arlot et al. 2010).

The performance of cross-validation-like procedures is typically characterized by an oracle inequality that bounds the error of the selected model. In a general cross-validation framework,

2

Van Der Laan & Dudoit (2003), van der Laan et al. (2004) provides finite sample oracle inequalities assuming that cross-validation is performed over a finite model class and Lecué et al. (2012) uses an entropy approach to bound the error for cross-validated models from potentially infinite model classes. In the regression setting, Györfi et al. (2006) provides a finite sample inequality for training/validation split for least squares and Wegkamp (2003) proves an oracle inequality for a penalized least squares holdout procedure. There are also bounds for cross-validated models from ridge regression and lasso (Golub et al. 1979, Chetverikov & Liao 2016, Chatterjee & Jafarov 2015), though the proofs usually rely on the linearity of the model class and are therefore hard to generalize.

Despite the wealth of literature on cross-validation, there is very little work on characterizing the prediction error when the regularization method has multiple penalty parameters. A potential reason is that tuning multiple penalty parameters is computationally difficult; most regularization methods only have one or two tuning parameters (e.g. the Elastic Net and Sparse Group Lasso (Zou & Hastie 2003, Simon et al. 2013)). This computational hurdle has been addressed recently by using continuous optimization methods. For many penalized regression problems, the gradient of the validation loss with respect to the penalty parameters can be calculated using an implicit differentiation trick (Bengio 2000, Foo et al. 2008). Thus a gradient descent procedure can be used to tune the penalty parameters. For more general "hyperparameter selection" problems, one can use a gradient-free approach such as Bayesian optimization Snoek et al. (2012) or Nelder-Mead (CITE).

This paper provides a finite-sample upper bound on the prediction error when multiple penalty parameters are tuned via a training/validation split or cross-validation. We establish an upper bound on the model error that depends on the oracle error and a near-parametric term. Roughly speaking, the additional price for not knowing the oracle penalty parameters is a parametric term. For semi- and non-parametric regression problems, this term is generally much smaller than the oracle error and do not affect the asymptotic convergence rate. In fact, in these cases, the number of penalty parameters can grow with the sample size. Our oracle inequalities depend on the assumption that the fitted models are smoothly parameterized by the penalty parameters. We will show that this smoothness assumption can be easily satisfied if we add a ridge penalty to the training criterion.

Section 2 provides bounds on the prediction error for a training/validation framework and cross-validation. Section 3 gives examples of penalized regression problems where the fitted models are smoothly parameterized by the penalty parameters. Section 4 provides a simulation study to support our theoretical results. Section 5 discusses our findings and potential future work. Section 6 contains the proofs and other technical details.

2 Main Result

2.1 Training/Validation Split

Given the total observed dataset D of size n, suppose it is randomly split into a training set T of size n_T and validation set V of size n_V. For a function h, define $\|h\|_V^2 = \frac{1}{n_V} \sum_{i \in V} h^2(x_i)$ and similarly for T. Using this notation, the fitted model defined in (2) can be written as

$$\hat{g}(\cdot|\boldsymbol{\lambda}) = \arg \min_{g \in \mathcal{G}} \frac{1}{2} \|y - g\|_T^2 + \sum_{j=1}^{J} \lambda_j P_j(g) \tag{3}$$

In the training/validation framework, we minimize the validation error by tuning over the range of possible penalty parameters values Λ. The selected penalty parameter can be expressed as

$$\hat{\boldsymbol{\lambda}} = \arg \min_{\boldsymbol{\lambda} \in \Lambda} \frac{1}{2} \|y - \hat{g}(\cdot|\boldsymbol{\lambda})\|_V^2 \tag{4}$$

We are interested in comparing its performance to the oracle penalty parameters $\tilde{\boldsymbol{\lambda}}$, which minimizes the model error as follows

$$\tilde{\boldsymbol{\lambda}} = \arg \min_{\boldsymbol{\lambda} \in \Lambda} \frac{1}{2} \|g^* - \hat{g}(\cdot|\boldsymbol{\lambda})\|_V^2 \tag{5}$$

We will establish a sharp oracle inequality for the model over the observed covariates in the validation set. Our bound is based on the basic inequality (van de Geer 2000). Let the set of fitted models be denoted

$$\mathcal{G}(T) = \{\hat{g}(\cdot|\boldsymbol{\lambda}) : \lambda \in \Lambda\} \tag{6}$$

From the definition of $\hat{\boldsymbol{\lambda}}$, we have

$$\left\| \hat{g}(\cdot|\hat{\boldsymbol{\lambda}}) - g^* \right\|_V^2 \;\leq\; \left\| \hat{g}(\cdot|\tilde{\boldsymbol{\lambda}}) - g^* \right\|_V^2 + 2 \left\langle \epsilon, \hat{g}(\cdot|\hat{\boldsymbol{\lambda}}) - \hat{g}(\cdot|\tilde{\boldsymbol{\lambda}}) \right\rangle_V \tag{7}$$

$$\leq\; \left\| \hat{g}(\cdot|\tilde{\boldsymbol{\lambda}}) - g^* \right\|_V^2 + \sup_{g \in \mathcal{G}(T)} 2 \left\langle \epsilon, g - \hat{g}(\cdot|\tilde{\boldsymbol{\lambda}}) \right\rangle_V \tag{8}$$

4

where $\langle h, \ell \rangle_V = \frac{1}{n_V} \sum_{i \in V} h(x_i)\ell(x_i)$. The first term in the upper bound is the best error achievable in the model class $\mathcal{G}(T)$. In this paper, the model class is pre-defined so this term can be treated as fixed. Our primary interest is bounding the second term, which is the supremum of empirical processes.

The supremum of empirical processes can be bounded using the complexity of the model class $\mathcal{G}(T)$. Complexity can be measured in a number of ways; we will use metric entropy in this paper. A more thorough review of empirical process theory is presented in Section 6. In this section, we only concern ourselves with smoothly-parameterized functions. We define this more formally as follows:

Definition 1. *A function $f(\cdot|\boldsymbol{\lambda})$ is C-smoothly-parameterized by $\boldsymbol{\lambda}$ over Λ with respect to norm $\|\cdot\|$ if*

$$\|f(\cdot|\boldsymbol{\lambda}_1) - f(\cdot|\boldsymbol{\lambda}_2)\| \leq C\|\boldsymbol{\lambda}_1 - \boldsymbol{\lambda}_2\|_2 \forall \boldsymbol{\lambda}_1, \boldsymbol{\lambda}_2 \in \Lambda \tag{9}$$

(9) can also be viewed as a generalized Lipschitz condition for the functional case. Function classes that satisfy (9) have low metric entropy. Hence their empirical process terms are small with high probability.

In the penalized regression setting, we are interested in bounding the metric entropy of $\mathcal{G}(T)$. It is clear that the fitted functions $\hat{g}(\cdot|\boldsymbol{\lambda})$ are parameterized by $\boldsymbol{\lambda}$, but more work is required to show that they are *smoothly*-parameterized. We defer that discussion to Section 3, where we provide examples of penalized regression problems that satisfy 9.

We now present a sharp oracle inequality for the penalty parameters selected by a training/validation split. The result is a special case of Theorem 3.

Theorem 1. *Suppose that the error ϵ are sub-Gaussian random variables with expectation zero.*

Suppose $\Lambda = [\lambda_{\min}, \lambda_{\max}]^J$.

Suppose that if $\|\epsilon\|_T \leq 2\sigma$, then $\hat{g}(\cdot|\boldsymbol{\lambda})$ is C-smoothly-parameterized by $\boldsymbol{\lambda}$ over Λ with respect to $\|\cdot\|_V$.

Then there are universal constants $c_1, c_2 > 0$ and constants $c_3, c_4 > 0$ such that

$$Pr\left(\left\|\hat{g}(\cdot|\hat{\boldsymbol{\lambda}}) - g^*\right\|_V - \left\|\hat{g}(\cdot|\tilde{\boldsymbol{\lambda}}) - g^*\right\|_V \geq \delta \wedge \|\epsilon\|_V \leq 2\sigma \right)$$

$$\le c_3 \exp\left(-\frac{n_V \delta^4}{c_3^2 \left\|\hat{g}(\cdot|\tilde{\boldsymbol{\lambda}}) - g^*\right\|_V^2}\right) + c_3 \exp\left(-\frac{n_V \delta^2}{c_3^2}\right) + c_3 \exp\left(-\frac{n_T \delta^2}{c_3^2}\right)$$

where

$$\delta = c_1 \left(\frac{J \log(\lambda_{\max} C) + c_4}{n_V}\right)^{1/2} + c_2 \sqrt{\left(\frac{J \log(\lambda_{\max} C) + c_4}{n_V}\right)^{1/2} \left\|\hat{g}(\cdot|\tilde{\boldsymbol{\lambda}}) - g^*\right\|_V}$$

(Check this formula!)

Technically we would like to tune the penalty parameters over the entire range $\Lambda = \mathbb{R}_+^J$, but $\hat{g}(\cdot|\boldsymbol{\lambda})$ can be very ill-behaved under such general conditions. We can instead ensure that Λ includes the penalty parameter

$$\tilde{\boldsymbol{\lambda}}_{\mathbb{R}_+} = \arg \min_{\boldsymbol{\lambda} \in \mathbb{R}_+^J} \|g^* - \hat{g}(\cdot|\boldsymbol{\lambda})\|_V^2 \tag{10}$$

As shown in van de Geer (2000), $\tilde{\boldsymbol{\lambda}}_{\mathbb{R}_+}$ shrinks at polynomial rate $O_p(n^{-\omega})$ for some $\omega > 0$, so the lower limit of Λ just needs to shrink at a faster polynomial rate.

We will therefore apply Theorem 1 the special case where $\Lambda = [n^{-t_{min}}, n^{t_{max}}]^J$. *n* or n_V? Technically we should use *n* but it's ugly? When the range of Λ grows at a polynomial rate, we find that the $\hat{g}(\cdot|\boldsymbol{\lambda})$ from our examples in Section 3 are actually Cn^κ-smoothly-parameterized for some $\kappa \ge 0$. For ease of interpretation, we present the results in asymptotic notation this time:

Lemma 1. $\Lambda = [n_V^{-t_{min}}, n_V^{t_{max}}]^J$.

Suppose that if $\|\epsilon\|_T \le 2\sigma$, there are constants C, κ such that $\hat{g}(\cdot|\boldsymbol{\lambda}^{(1)})$ is Cn^κ-smoothly-parameterized by $\boldsymbol{\lambda}$ over Λ with respect to $\|\cdot\|_V$.

Then

$$\left\|\hat{g}(\cdot|\hat{\boldsymbol{\lambda}}) - g^*\right\|_V \le \quad \left\|\hat{g}(\cdot|\tilde{\boldsymbol{\lambda}}) - g^*\right\|_V \tag{11}$$

$$+ O_p \left(\frac{J(1 + t_{max} + \kappa) \log n_V}{n_V}\right)^{1/2} \tag{12}$$

$$+ O_p \left(\frac{J(1 + t_{max} + \kappa) \log n_V}{n_V}\right)^{1/4} \left\|\hat{g}(\cdot|\tilde{\boldsymbol{\lambda}}) - g^*\right\|_V^{1/2} \tag{13}$$

6

From Lemma 1, we see that the model error is upper bounded by the oracle error and a two-part remainder term: a near-parametric term in 12 and a geometric mean of the oracle error and 12.

The appearance of a near-parametric term makes intuitive sense. We are trying to estimate the oracle penalty parameters using the validation set, which roughly corresponds to solving a parametric regression problem. The reason we refer to 12 as near-parametric is that the convergence rate of a J-dimensional parametric regression problem is usually $(J/n)^{1/2}$ but 12 has a $\log n$ term in the numerator. The $\log n$ term was introduced when we allowed the range of Λ to grow with the sample size.

However, the appearance of the geometric mean suggests that treating the problem of tuning penalty parameters as a parametric regression problem is an oversimplification. We are truly solving the bi-level optimization problem:

$$\hat{\boldsymbol{\lambda}} = \arg \min_{\boldsymbol{\lambda} \in \Lambda} \frac{1}{2} \|y - \hat{g}(\cdot|\boldsymbol{\lambda})\|_V^2$$

$$\text{s.t. } \hat{g}(\cdot|\boldsymbol{\lambda}) = \arg \min_{g \in \mathcal{G}} \frac{1}{2} \|y - g\|_T^2 + \sum_{j=1}^{J} \lambda_j P_j(g)$$

For example, if the lower level optimization problem is non-parametric, the upper level optimization problem isn't truly parametric.

Now we consider the asymptotic behavior of model error. As long as the oracle error converges at a sub-parametric rate, the oracle error will dominate and the other two terms will be negligible. Therefore in these settings, we can actually allow the number of penalty parameters to grow with the sample size without affecting the asymptotic convergence rate. That is, we can allow the number of penalty parameters J grow at the rate

$$J = O_p \left(\frac{\left\| g^* - \hat{g}(\cdot|\tilde{\boldsymbol{\lambda}}) \right\|_V^2}{\left(\frac{J(1 + t_{max} + \kappa) \log n_V}{n_V} \right)^{1/2}} \right) \tag{14}$$

On the other hand, if the oracle error converges at a parametric rate, we have to keep the number of penalty parameters fixed.

2.2 Cross-Validation

In this section, we give an oracle inequality for K-fold cross-validation. Instead of bounding the model error over the observed covariates, we will bound the generalization error, which is the squared $L2$-norm of the difference:

$$\|g - g^*\|^2 = \int |g(x) - g^*(x)|^2 \, dx \tag{15}$$

Toward this end, we will apply the oracle inequality in Lecué et al. (2012).

We will generalize the notation from the previous section. Let a dataset with n samples be denoted $D^{(n)}$. The fitted model given any training data $D^{(n)}$ is denoted

$$\hat{g}_{D^{(n)}}(\cdot|\boldsymbol{\lambda}) = \arg\min_{g \in \mathcal{G}} \frac{1}{2}\|y - g\|^2_{D^{(n)}} + \sum_{j=1}^{J} \lambda_j P_j(g) \tag{16}$$

For K-fold cross-validation, the problem setup is as follows. As before, let $D^{(n)}$ be the entire dataset. For simplicity, suppose the dataset can be partitioned into K sets of equal size n_V. Let $n_T = n - n_V$. Then partition k will be denoted $D_k^{(n_V)}$ and its complement will be denoted $D_{-k}^{(n_T)} = D \setminus D_k^{(n_V)}$. The selected penalty parameters is

$$\hat{\boldsymbol{\lambda}} = \arg\min_{\boldsymbol{\lambda} \in \Lambda} \frac{1}{2K} \sum_{k=1}^{K} \left\| y - \hat{g}_{D_{-k}^{n_T}}(\cdot|\boldsymbol{\lambda}) \right\|^2_{D_k} \tag{17}$$

In traditional cross-validation, the final model is retrained on all the data with $\hat{\boldsymbol{\lambda}}$. However, bounding its generalization error requires additional regularity assumptions (Lecué et al. 2012). We consider the following "averaged version of cross-validation" instead

$$\bar{g}_{D^n}(x) = \frac{1}{K} \sum_{k=1}^{K} \hat{g}_{D_{-k}^{(n_T)}}(x|\hat{\boldsymbol{\lambda}}) \tag{18}$$

The following theorem bounds the generalization error of $\bar{g}_{D^n}$.

Theorem 2. *Suppose the error ϵ are sub-Gaussian random variables with expectation zero. Suppose $\sup_{g \in \mathcal{G}} \|g\|_\infty \leq G$.*

Suppose $\Lambda = [\lambda_{\min}, \lambda_{\max}]^J$.

Suppose that if $\|\epsilon\|_T \leq 2\sigma$, there exist constants C such that for any dataset D^{n_T}, $\hat{g}_{D^{n_T}}(\cdot|\boldsymbol{\lambda})$ is C-smoothly-parameterized by $\boldsymbol{\lambda}$ over Λ with respect to $\|\cdot\|_\infty$.

For all $a > 0$,

$$E_{D^{(n)}} \|\bar{g}_{D^n} - g^*\|^2 \leq (1+a) \min_{\boldsymbol{\lambda} \in \Lambda} E_{D^{(n_T)}} \|\hat{g}_{D^{(n_T)}}(\cdot|\boldsymbol{\lambda}) - g^*\|^2 + \frac{c_a}{n_V} \left(complicated \log n term\right) \tag{19}$$

where c_a is some constant.

There are some clear differences between Theorems 1 and 2. Theorem 2 allows us to bound the generalization error, but it comes at a price. One, it requires that the fitted functions are smoothly parameterized by $\boldsymbol{\lambda}$ over the entire domain. In addition, Theorem 2 is no longer a strict oracle inequality since the oracle error is scaled by the constant $1 + a$.

Now we apply Theorem 2 to the special case where Λ grows at a polynomial rate with the sample size. We will use the same assumptions as we did in Lemma 1.

Lemma 2. *Suppose $\sup_{g \in \mathcal{G}} \|g\|_\infty \leq G$.*

Suppose $\Lambda = [n^{-t_{\min}}, n^{t_{\max}}]^J$.

Suppose that if $\|\epsilon\|_T \leq 2\sigma$, there are constants C, κ such that for any dataset $D^{(n_T)}$, $\hat{g}_{D^{(n_T)}}(\cdot|\boldsymbol{\lambda})$ is Cn^κ-smoothly-parameterized by $\boldsymbol{\lambda}$ over Λ with respect to $\|\cdot\|_\infty$.

For all $a > 0$,

$$E_{D^{(n)}} \|\bar{g}_{D^{(n)}} - g^*\|^2 \leq (1+a) \min_{\boldsymbol{\lambda} \in \Lambda} E_{D^{(n_T)}} \|\hat{g}_{D^{(n_T)}}(\cdot|\boldsymbol{\lambda}) - g^*\|^2 + c_a \left(\frac{\log(n_V) + \log(n_T) + stuff}{n_V}\right) \tag{20}$$

Lemmas 2 and 1 are quite similar in that the upper bounds are functions of the oracle error and a near-parametric term. The asymptotic convergence rate of the selected model is determined by whichever term dominates. For both the training/validation split framework and cross-validation, we find that tuning penalty parameters is a relatively "cheap" problem to solve. If the oracle error is sub-parametric, the cost of tuning penalty parameters is negligible asymptotically.

The theorems and lemmas given in this section are all finite-sample results. One could try to minimize the upper bound by increasing the number of penalty parameters or changing the ratio between the training and validation set sizes. Determining the optimal number of penalty parameters will unfortunately require knowing characteristics about the error variables ϵ. (Perhaps you can use cross-validation to determine the number of penalty parameters to use. Ha! How meta!)

3 Smoothness of $\hat{g}(\cdot|\boldsymbol{\lambda})$ in $\boldsymbol{\lambda}$

Theorem 1 and 2 require the fitted functions $\hat{g}(\cdot|\boldsymbol{\lambda})$ to be smoothly parametrized by $\boldsymbol{\lambda}$ as defined in (9). We now present examples of penalized regression problems where these conditions are satisfied. Recall that Theorem 1 requires smoothness with respect to $\|\cdot\|_V$ whereas Theorem 2 requires smoothness with respect to $\|\cdot\|_\infty$. Therefore any example that satisfies the smoothness condition for Theorem 2 also satisfies the smoothness condition for Theorem 1.

Throughout, we will presume that $\mathcal{G}$ is a convex function class.

3.1 Smoothness over the Validation Set

Theorem 1 requires that $\hat{g}(\cdot|\boldsymbol{\lambda})$ is C-smoothly-parameterized by $\boldsymbol{\lambda}$ over Λ with respect to $\|\cdot\|_V$. We show that nonparametric additive models satisfy this smoothness condition.

Penalized regression problems for additive models usually minimize a training criterion of the following form

$$\{\hat{g}_j(\cdot|\boldsymbol{\lambda})\}_{j=1}^J = \arg\min_{g\in\mathcal{G}} \left\| \boldsymbol{y} - \sum_{j=1}^J g_j(\boldsymbol{x}_j) \right\|_T^2 + \sum_{j=1}^J \lambda_j P_j(g_j) \tag{21}$$

Instead of dealing with (21) directly, we consider minimizers of the perturbed training criterion

$$\{\hat{g}_j(\cdot|\boldsymbol{\lambda})\}_{j=1}^J = \arg\min_{g\in\mathcal{G}} \left\| \boldsymbol{y} - \sum_{j=1}^J g_j(\boldsymbol{x}_j) \right\|_T^2 + \sum_{j=1}^J \lambda_j \left(P_j(g_j) + \frac{w}{2}\|g_j\|_D^2 \right) \tag{22}$$

(22) has an additional ridge penalty for each of the additive components, where each of the ridge penalties is scaled by a fixed constant $w > 0$.

For both this example and the one in Section 3.2, we perturb the penalized regression problems with additional ridge penalties scaled by a constant w. The ridge penalty is primarily for the proofs to carry through; it ensures that the fitted functions are "well-conditioned." In practice, w can be chosen small enough that the fitted models for the original problem and the perturbed ridge problem are indistinguishable. In addition, we show in Lemma 7 that for parametric regression problems that are strongly convex, the effect of the ridge penalty is negligible. Of course we would like to do without the ridge penalty, but one will probably need more assumptions about the penalized regression problem.

We will consider the case where the penalty functions P_j are convex and twice-differentiable. In the nonparametric setting, we will need the concept of pathwise differentiability:

Definition 2. *Let $\mathcal{G}$ be a function class. Let $P : \mathcal{G} \mapsto \mathbb{R}$ be a functional and g and h be functions in $\mathcal{G}$. The pathwise derivative of P at g with respect to h is defined as*

$$\frac{d}{dm}P(g + mh) = \lim_{m \to 0} \frac{P(g + mh) - P(g)}{m}$$

if the limit exists. The pathwise second derivative of P at g with respect to h is defined as

$$\frac{d^2}{dm^2}P(g + mh) = \lim_{m \to 0} \frac{\frac{d}{dt}P(g + th) - \frac{d}{dm}P(g)}{m}$$

if the pathwise derivative of P and the limit exists. P is twice-differentiable if the pathwise second derivative of P at any $g \in \mathcal{G}$ with respect to any $h \in \mathcal{G}$ exists.

Furthermore, one can show that the functional P is convex if the pathwise second derivative of a penalty function is always positive as follows

$$\frac{d^2}{dm^2}P_j(f + mh) \geq 0 \forall j = 1, ..., J \text{ and } \forall h \in \mathcal{G} \tag{23}$$

(Do I need to prove or define this? Has someone done this already?).

As an example, consider the r-th degree Sobolev penalty

$$P(g) = \int \left(g^{(r)}(x)\right)^2 dx \tag{24}$$

Its pathwise second derivative at g with respect to h is

$$\frac{d^2}{dm^2}P(g) = \frac{d^2}{dm^2}\int \left((g + mh)^{(r)}(x)\right)^2 dx \tag{25}$$

$$= 2\int \left(h^{(r)}(x)\right)^2 dx \tag{26}$$

The following lemma states that the fitted functions from 22 are smoothly parameterized by the penalty parameters.

Lemma 3. *Consider $\hat{g}_j(\cdot|\boldsymbol{\lambda})$ as defined in 22. Suppose the penalty functions P_j is twice-differentiable and convex.*

Suppose $\Lambda = [\lambda_{\min}, \lambda_{\max}]^J$.

For all $\boldsymbol{\lambda}^{(1)}, \boldsymbol{\lambda}^{(2)} \in \Lambda$, we have

$$\left\| \sum_{j=1}^{J} \hat{g}_j(\cdot | \boldsymbol{\lambda}^{(1)}) - \hat{g}_j(\cdot | \boldsymbol{\lambda}^{(2)}) \right\|_V \leq \left\| \boldsymbol{\lambda}^{(1)} - \boldsymbol{\lambda}^{(2)} \right\| stuff$$

where stuff depends on $\|\epsilon\|_T$.

All of the proofs on the smoothness of $\hat{g}(\cdot | \boldsymbol{\lambda})$ follow the same recipe. The first step is to consider the optimization problem (21) restricted to models on the line

$$\left\{ \hat{g}(\cdot | \boldsymbol{\lambda}^{(1)}) + m \left(\hat{g}(\cdot | \boldsymbol{\lambda}^{(2)}) - \hat{g}(\cdot | \boldsymbol{\lambda}^{(1)}) \right) : m \in [0, 1] \right\} \tag{27}$$

By implicit differentiation of the KKT conditions, we can then determine how the fitted models change with respect to the penalty parameters. Finally, the difference $\|\hat{g}(\cdot | \boldsymbol{\lambda}^{(1)}) - \hat{g}(\cdot | \boldsymbol{\lambda}^{(2)})\|$ is bounded using the mean value theorem.

For illustration, we present the proof for Lemma 3 in the case where there is only one penalty parameter. The case with multiple penalty parameters is given in Section 6.

Proof of Lemma 3. Let $h = \hat{g}(\cdot | \lambda^{(1)}) - \hat{g}(\cdot | \lambda^{(2)})$. Suppose for contradiction that $\|h\|_D > d$. Consider the one-dimensional optimization problem

$$\hat{m}(\lambda) = \arg\min_m \frac{1}{2} \|y - (g + mh)\|_T^2 + \lambda \left(P(g + mh) + \frac{w}{2} \|g + mh\|_D^2 \right)$$

Now by the KKT conditions, we have

$$\langle y - (g + mh), h \rangle_T + \lambda \frac{\partial}{\partial m} P(g + mh) + \lambda w \langle h, g + mh \rangle_D = 0$$

It's implicit derivative with respect to λ is

$$\frac{\partial \hat{m}(\lambda)}{\partial \lambda} = \left(\|h\|_T^2 + \lambda \frac{\partial^2}{\partial m^2} P(g + mh) + \lambda w \|h\|_D^2 \right)^{-1} \left(\frac{\partial}{\partial m} P(g + mh) + w \langle h, g + mh \rangle_D \right) \tag{28}$$

By the KKT conditions and the definitions of $\hat{m}(\lambda)$, e can show

$$\left| \frac{\partial}{\partial m} P(g + mh) \right|_{m = \hat{m}(\lambda)} \leq C \|h\|_D$$

and

$$w \langle h, g + mh \rangle_D |_{m = \hat{m}(\lambda)} \leq C \|h\|_D$$

for some constant C. Hence

$$\left|\frac{\partial}{\partial\lambda}\hat{m}(\lambda)\right| \le 2C(\lambda_{\min}w)^{-1}\|h\|_D^{-1}$$

By the MVT, there is some $\alpha \in (\lambda^{(1)}, \lambda^{(2)})$ such that

$$
\begin{aligned}
\left|\hat{m}(\lambda^{(2)}) - \hat{m}(\lambda^{(1)})\right| &= \left|\left(\lambda^{(2)} - \lambda^{(1)}\right)\left.\frac{\partial\hat{m}(\lambda)}{\partial\lambda}\right|_{\lambda=\alpha}\right| \\
&\le |\lambda^{(2)} - \lambda^{(1)}|2C(\lambda_{\min}w)^{-1}\|h\|_D^{-1}
\end{aligned}
$$

Since we know that $\hat{m}(\lambda^{(2)}) = 1$ and $\hat{m}_{\tilde{k}}(\lambda^{(1)}) = 0$, we can rearrange the inequality to get our final result. $\qquad\square$

3.2 Smoothness over the entire domain

Theorem 2 requires the fitted functions to be smoothly-parameterized by the penalty parameters with respect to $\|\cdot\|_\infty$. This is difficult to show for nonparametric estimators. Instead we will consider parametric models where the number of dimensions to grow with n, as commonly done in sieve estimation.

In the previous section, we assumed the nonparametric penalties were smooth. Here, we can lift this restriction and consider non-smooth penalties like the lasso and the group lasso.

3.2.1 Parametric Regression with smooth penalties

Consider the parametric regression setting where the model parameters have dimension p. We will assume the penalty functions are smooth for now. Given the original penalized regression problem

$$\hat{\boldsymbol{\theta}}(\boldsymbol{\lambda}) = \underset{\boldsymbol{\theta}\in\mathbb{R}^p}{\arg\min}\|y - g(X|\boldsymbol{\theta})\|_T^2 + \sum_{j=1}^J \lambda_j\left(P_j(\boldsymbol{\theta})\right) \tag{29}$$

we again perturb the problem with additional ridge penalties

$$\hat{\boldsymbol{\theta}}(\boldsymbol{\lambda}) = \underset{\boldsymbol{\theta}\in\mathbb{R}^p}{\arg\min}\|y - g(X|\boldsymbol{\theta})\|_T^2 + \sum_{j=1}^J \lambda_j\left(P_j(\boldsymbol{\theta}) + \frac{w}{2}\|\boldsymbol{\theta}\|_2^2\right) \tag{30}$$

In contrast to (22), the ridge penalty is on the model parameters rather than the fitted values.

Notice that in Section 3.1, we considered an additive model. In this section, we will consider a model with multiple penalties that are scaled individually. One can also show that

a parametric additive model with an additional ridge penalty $\|\theta_j\|_2^2$ satisfies the smoothness condition. The proof for the parametric additive models is very similar to that for Lemma 3.

We can show smoothness over the entire domain under the following conditions

Condition 1. *There exists some constant K such that for penalty function P_j for all $j = 1, ..., j,$*

$$\frac{d}{dm}P(\boldsymbol{\theta} + m\boldsymbol{\beta}) \le K\|\boldsymbol{\beta}\|_2 \tag{31}$$

for any $\boldsymbol{\theta}, \boldsymbol{\beta} \in \mathbb{R}^p$.

Condition 2. *There exist constants $L, r \ge 0$ such that the functions are Lp^r-smoothly-parameterized in the model parameters with respect to $\|\cdot\|_\infty$:*

$$\|g(\cdot|\boldsymbol{\theta}^{(1)}) - g(\cdot|\boldsymbol{\theta}^{(2)})\|_\infty \le Lp^r\|\boldsymbol{\theta}^{(1)} - \boldsymbol{\theta}^{(2)}\|_2 \forall \boldsymbol{\theta}^{(1)}, \boldsymbol{\theta}^{(2)} \in \mathbb{R}^p \tag{32}$$

It is easy to show that Condition 1 is satisfied by many popular parametric penalties, such as the ridge penalty $\|\cdot\|_2^2$, lasso $\|\cdot\|_1$, and group lasso $\|\cdot\|_2$. (Proofs are given in Section 6, if you insist.)

Condition 2 requires that the smoothness constant grows at a polynomial rate in the number of features. Many models satisfy this condition, assuming they are parameterized appropriately. For example, Condition 2 is satisfied by linear regression when the covariates are bounded. With these assumptions, we can show that the fitted values are smooth with respect to the penalty parameters over the entire domain. Note that the remainder term in Lemma 1 and 2 remains near-parametric if p grows at some polynomial rate in n.

The following lemma states that for penalized regression problems as in (30), the fitted models are smoothly parameterized by the penalty parameters. The proof follows the outline given in Section 3.1.

Lemma 4. *Suppose Condition 1 and 2 are satisfied. Suppose $\hat{\boldsymbol{\theta}}$ is defined by (30). For any $\boldsymbol{\lambda}^{(1)}, \boldsymbol{\lambda}^{(2)} \in \Lambda$, we have*

$$\left\|g\left(\cdot|\hat{\boldsymbol{\theta}}(\boldsymbol{\lambda}^{(1)})\right) - g\left(\cdot|\hat{\boldsymbol{\theta}}(\boldsymbol{\lambda}^{(2)})\right)\right\|_\infty \le \left\|\boldsymbol{\lambda}^{(2)} - \boldsymbol{\lambda}^{(1)}\right\|_2 stuff$$

3.2.2 Nonsmooth penalties

If the regression problem contains non-smooth penalty functions, similar results do not necessarily hold. Nonetheless, we find that for many popular non-smooth penalty functions, the fitted functions are still smoothly parameterized by $\boldsymbol{\lambda}$ almost everywhere. To characterize such problems, we use the approach in Feng & Simon (TBD- CITE?). We begin with the following definitions:

Definition 3. *The differentiable space of a real-valued function L at $\boldsymbol{\theta}$ is the set of functions*

$$\Omega^L(\boldsymbol{\theta}) = \left\{ \boldsymbol{\beta} \,\bigg|\, \lim_{\epsilon \to 0} \frac{L(\boldsymbol{\theta} + \epsilon\boldsymbol{\beta}) - L(\boldsymbol{\theta})}{\epsilon} \ \text{exists} \right\} \tag{33}$$

Definition 4. *S is a local optimality space for a convex function $L(\cdot, \boldsymbol{\lambda}_0)$ if there exists a neighborhood W containing $\boldsymbol{\lambda}_0$ such that for every $\boldsymbol{\lambda} \in W$,*

$$\arg\min_{\boldsymbol{\theta} \in \mathbb{R}^p} L(\boldsymbol{\theta}, \boldsymbol{\lambda}) = \arg\min_{\boldsymbol{\theta} \in S} L(\boldsymbol{\theta}, \boldsymbol{\lambda}) \tag{34}$$

We now use these definitions to state the conditions that guarantee that the fitted functions are still smoothly parameterized by the penalty parameters. Let the training criterion be denoted

$$L_T(\boldsymbol{\theta}, \boldsymbol{\lambda}) \;=\; \arg\min_{g \in \mathcal{G}} \|\boldsymbol{y} - g(X|\boldsymbol{\theta})\|_T^2 + \sum_{j=1}^J \lambda_j \left(P_j(\boldsymbol{\theta}) + \frac{w}{2}\|\boldsymbol{\theta}\|_D^2 \right)$$

We will need following conditions to hold for almost every $\boldsymbol{\lambda} \in \Lambda$:

Condition 3. *The differentiable space $\Omega^{L_T(\cdot, \boldsymbol{\lambda})}(\boldsymbol{\theta})$ at $\hat{\boldsymbol{\theta}}(\boldsymbol{\lambda})$ is a local optimality space for $L_T(\cdot, \boldsymbol{\lambda})$.*

Condition 4. *$L_T(\cdot, \boldsymbol{\lambda})$ is twice continuously differentiable along directions in $\Omega^{L_T(\cdot, \boldsymbol{\lambda})}(\hat{\boldsymbol{\theta}}(\boldsymbol{\lambda}))$.*

Equipped with the conditions above, we can characterize the smoothness of the fitted functions when the penalties are non-smooth. In fact the result is exactly the same as Lemma 3.

Lemma 5. *Suppose that $\sup_{g \in \mathcal{G}} \|g\|_D \leq G$. Suppose $\lambda_j \geq \lambda_{\min}$ for all j. Suppose the penalty functions are convex. Suppose Conditions 1 and 2 hold for almost every $\boldsymbol{\lambda}$. Suppose Conditions 3 and 4 are satisfied for almost every $\boldsymbol{\lambda} \in \Lambda$.*

For any $\boldsymbol{\lambda}^{(1)}, \boldsymbol{\lambda}^{(2)} \in \Lambda$, we have

$$\left\| g\left(\cdot | \hat{\boldsymbol{\theta}}(\boldsymbol{\lambda}^{(1)})\right) - g\left(\cdot | \hat{\boldsymbol{\theta}}(\boldsymbol{\lambda}^{(2)})\right) \right\|_V \leq \left\| \boldsymbol{\lambda}^{(1)} - \boldsymbol{\lambda}^{(2)} \right\| stuff$$

3.3 Example: Smoothing Splines with a Sobolev Penalty

Finally, we consider the example of smoothing splines fitted using the Sobolev penalty (De Boor et al. 1978, Wahba 1990, Green & Silverman 1994). For a given set of penalty parameters, the smoothing spline estimate is

$$\{\hat{g}_j(\cdot|\boldsymbol{\lambda})\}_{j=1}^J = \arg\min_{g_j \in \mathcal{G}} \frac{1}{2} \left\| y - \sum_{j=1}^J g_j \right\|_T^2 + \sum_{j=1}^J \lambda_j \int \left(g_j^{(r_j)}(x) \right)^2 dx \tag{35}$$

where $g^{(r)}$ is the derivative of g of order $r \geq 2$.

We can show that smoothing splines are smoothly-parameterized by the penalty parameters with respect to $\| \cdot \|_V$ using the approach in Section 3.1. As done in the nonparametric additive model example, we can perturb (35) with an additional ridge penalty as follows

$$\{\hat{g}_j(\cdot|\boldsymbol{\lambda})\}_{j=1}^J = \arg\min_{g_j \in \mathcal{G}} \frac{1}{2} \left\| y - \sum_{j=1}^J g_j \right\|_T^2 + \sum_{j=1}^J \lambda_j \left(\int \left(g_j^{(r_j)}(x) \right)^2 dx + \frac{w}{2} \|g_j\|_D^2 \right) \tag{36}$$

Moreover, solutions to (35) have the property that the fitted functions $\hat{g}_j(\cdot|\boldsymbol{\lambda})$ can be expressed as the weighted sum of normalized B-splines: (CITE for proof)

$$\hat{g}_j(x|\boldsymbol{\lambda}) = \sum_{i=1}^p \theta_i N_{ij}(x) \tag{37}$$

where N_{ij} is a normalized B-spline. The degree of B-spline depends on the degree of the Sobolev penalty and the number of B-splines p is determined by the number of knots and the degree of the B-spline. Since smoothing splines are parametric, we can then apply the same logic in Section 3.2 to show that smoothing splines are smoothly-parameterized by the penalty parameters with respect to $\| \cdot \|_\infty$. Again, we perturb (35) with an additional ridge penalty as follows

$$\{\hat{g}_j(\cdot|\boldsymbol{\lambda})\}_{j=1}^J = \arg\min_{g_j \in \mathcal{G}} \frac{1}{2} \left\| y - \sum_{j=1}^J N_j \boldsymbol{\theta}_j \right\|_T^2 + \sum_{j=1}^J \lambda_j \left(P_j(\boldsymbol{\theta}_j) + \frac{w}{2} \|\boldsymbol{\theta}_j\|_D^2 \right) \tag{38}$$

The key is to show that Condition 3 is satisfied.

The following lemma states that smoothing splines are indeed smoothly-parameterized by the penalty parameters.

Lemma 6. *Suppose* $\sup_{g \in \mathcal{G}} \|g\|_\infty \leq G$.

Suppose $\lambda_j \in [\lambda_{\min}, \lambda_{\max}]^J$ *for all* $j = 1, ..., j$.

In the setting of (36)*, the fitted functions satisfy*

$$\left\| \sum_{j=1}^J \hat{g}_j(\cdot|\lambda^{(1)}) - \hat{g}_j(\cdot|\lambda^{(2)}) \right\|_V \leq \left\| \lambda^{(1)} - \lambda^{(2)} \right\| stuff \tag{39}$$

In the setting of (38)*, the fitted functions satisfy*

$$\left\| \sum_{j=1}^J \hat{g}_j(\cdot|\lambda^{(1)}) - \hat{g}_j(\cdot|\lambda^{(2)}) \right\|_\infty \leq \left\| \lambda^{(1)} - \lambda^{(2)} \right\| stuff \tag{40}$$

4 Simulations

We now provide a simulation study for the prediction error bound given in Theorem 3. The penalty parameters are chosen by a training/validation split. We show that the error of the select model converges to that of the oracle model at the expected $(\log(n_V)/n_V)^{1/2}$ rate.

Observations were generated from the model

$$y = sin(x_1) + \frac{1}{2} sin(2x_2 + 1) + \sigma\epsilon \tag{41}$$

where $\epsilon \sim N(0,1)$ and σ scaled the error term such that the signal to noise ratio was 2. The covariates x_1 and x_2 were uniformly distributed over the interval $(0,6)$. Smoothing splines were fit with a Sobolev penalty

$$\hat{g}_{1,\lambda}, \hat{g}_{2,\lambda} = \underset{g_1, g_2}{\arg\min} \|y - f_1(x_1) - f_2(x_2)\|_T^2 + \int_0^6 (f_1^{(2)}(x))^2 dx + \int_0^6 (f_2^{(2)}(x))^2 dx \tag{42}$$

The training set contained 100 samples and models were fitted with 10 knots. A grid search was performed over the penalty parameter values $\{10^{-6+0.2i} : i = 0, ..., 25\}$. We tested validation set sizes $n_V = 20, 30, ..., 80$. The oracle penalty parameters were chosen by minimizing the difference between the fitted model and the true model over a separate test set of 800 samples. A total of 30 simulations were run for each validation set size.

Figure 4 plots the validation loss $\|\hat{g}_\lambda - g^*\|_V$ of the model tuned using a validation set versus the model fit using the oracle penalty parameters. As the validation set increases, the error of the tuned model converges towards the oracle model as expected. In addition

Figure 1:   Validation loss difference between oracle and selected model as validation set size grows
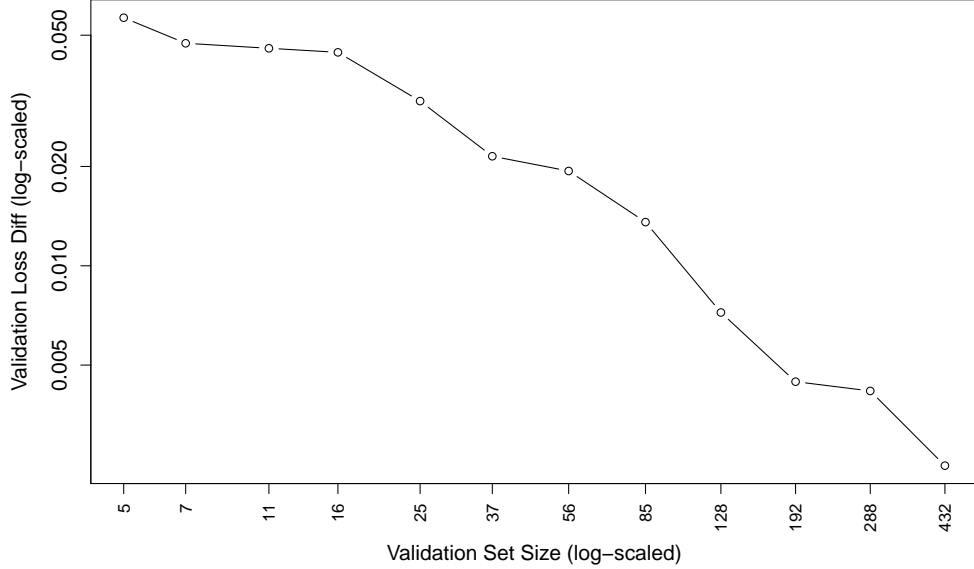
we compare the observed difference between the validation losses for the two models and the expected convergence rate of $O_p\left(n_V^{-1/4}\right)$. (Note that all other factors that influence the convergence rate are constant since we only vary the validation set size.) The plot shows that theory closely matches the empirical evidence.

5   Discussion

In this paper, we have shown that the difference in prediction error of the model chosen by cross-validation and the oracle model decreases at a near-parametric rate if the fitted models are smoothly parameterized in terms of the penalty parameters. For many penalized regression problems, we find that this is indeed the case. Our results show that adding penalty parameters does not drastically increase the model complexity. This supports recent efforts to combine regularization methods and "un-pool" regularization parameters. Furthermore, since our result holds for a search over a dense set of penalty parameters, our prediction error bounds apply to cross-validation over a continuum of values, as done in hyper-parameter optimization methods.

The main caveat is that our theorems bound the prediction error of the global minimizer

of the validation set. However this is hard to achieve practically since the validation loss is not convex in the penalty parameters. More investigation needs to be done to bound the prediction error of fitted models that are local minima.

A different approach we could have taken in this paper is to bound the distance between the estimated and oracle penalty parameters

$$\left\| \hat{\boldsymbol{\lambda}} - \tilde{\boldsymbol{\lambda}} \right\|_2 \tag{43}$$

instead of the fitted values. Bounding 43 is not obvious from the definitions of $\hat{\boldsymbol{\lambda}}$ and would probably require more regularity assumptions on the model class. However, it could provide a more intuitive understanding of the behavior of cross-validation-like procedures.

6 The Proof

In this paper, we will measure the the complexity of $\mathcal{G}(T)$ by its metric entropy. Let us recall its definition here:

Definition 5. *Let the covering number $N(u, \mathcal{G}, \|\cdot\|)$ be the smallest set of u-covers of $\mathcal{G}$ with respect to the norm $\|\cdot\|$. The metric entropy of $\mathcal{G}$ is defined as the log of the covering number:*

$$H(u, \mathcal{G}, \|\cdot\|) = \log N(u, \mathcal{G}, \|\cdot\|) \tag{44}$$

Theorem 3. *Let ϵ be independent sub-Gaussian random variables. Suppose that $\sup_{g \in \mathcal{G}} \|g\|_\infty \leq G < \infty$. Suppose for any training dataset $T \subseteq D$ with $\|\epsilon\|_T \leq 2\sigma$, we have*

$$\int_0^R H^{1/2}\left(u, \mathcal{G}(\cdot|\mathcal{T})\|\cdot\|_V\right) du \leq \psi(n, J, \sigma) \tag{45}$$

Then for all $\delta > 0$ such that

$$\sqrt{n_V} \delta^2 \geq c \left[\psi_T \left(2 \left\| \hat{g}_{\tilde{\lambda}} - g^* \right\|_V + 2\delta \right) \vee \left(2 \left\| \hat{g}_{\tilde{\lambda}} - g^* \right\|_V + 2\delta \right) \right] \tag{46}$$

Then with high probability, we have

$$\|\hat{g}_{\hat{\lambda}}(\cdot|T) - g^*\|_V \leq \min_{\lambda \in \Lambda} \|\hat{g}_\lambda(\cdot|T) - g^*\|_V + \delta \tag{47}$$

Proof. Chaining and peeling. $\qquad\square$

Proof of Theorem 1

Proof. □

Proof of Theorem 2

Lemma 7. *The oracle rate isn't changed when we add the ridge penalty*

Proof of Lemma 3

Proof of Lemma 5

Proof of Lemma 4

Lemma 8. *Sobolev penalty has nice properties*

Proof of Lemma 6

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