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# One-step estimator paths for concave regularization

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## Abstract

The statistics literature of the past 15 years has established many favorable properties for sparse diminishing-bias regularization: techniques which can roughly be understood as providing estimation under penalty functions spanning the range of concavity between  $L_0$  and  $L_1$  norms. However, lasso  $L_1$ -regularized estimation remains the standard tool for industrial ‘Big Data’ applications because of its minimal computational cost and the presence of easy-to-apply rules for penalty selection. In response, this article proposes a simple new algorithm framework that requires no more computation than a lasso path: the path of one-step estimators (POSE) does  $L_1$  penalized regression estimation on a grid of decreasing penalties, but adapts coefficient-specific weights to decrease as a function of the coefficient estimated in the previous path step. This provides sparse diminishing-bias regularization at no extra cost over the fastest lasso algorithms. Moreover, our ‘gamma lasso’ implementation of POSE is accompanied by a reliable heuristic for the fit degrees of freedom, so that standard information criteria can be applied in penalty selection. The methods are illustrated in extensive simulations and in application of logistic regression to evaluating the performance of hockey players.

## 1 Introduction

For regression in high-dimensions, it is useful to regularize estimation through a penalty on coefficient size.  $L_1$  regularization (i.e., the lasso of Tibshirani, 1996) is especially popular, with costs that are non-differentiable at their minima and can lead to coefficient solutions of exactly zero. A related approach is concave penalized regularization (e.g. SCAD from Fan and Li 2001 or MCP from Zhang 2010a) with cost functions that are also spiked at zero but flatten

for large values (as opposed to the constant increase of an  $L_1$  norm). This yields sparse solutions where large non-zero values are estimated with little bias.

The combination of *sparsity* and *diminishing-bias* is appealing in many settings, and a large literature on concave penalized estimation has developed over the past 15 years. For example, many authors (e.g., from Fan and Li 2001 and Fan and Peng 2004) have contributed work on their *oracle properties*, a class of results showing conditions under which coefficient estimates through concave penalization, or in related schemes, will be the same as if you knew the sparse ‘truth’ (either asymptotically or with high probability). From an information compression perspective, the increased sparsity encouraged by diminishing-bias penalties (since single large coefficients are allowed to account for the signals of other correlated covariates) leads to lower memory, storage, and communication requirements. Such savings are very important in distributed computing schemes (e.g., Taddy, 2013a).

Unfortunately, exact solvers for concave penalized estimation all require significantly more compute time than a standard lasso. This has precluded their use in settings – e.g., text or web-data analysis – where both  $n$  (the number of observations) and  $p$  (covariate dimension) are very large. As we review in Section 3, recent literature recommends the use of approximate solvers. These approximations take the form of iteratively-weighted- $L_1$  regularization, where the coefficient-specific weights are based upon results from previous iterations of the approximate solver. Work on one-step estimation (OSE), e.g. by Zou and Li (2008), shows that even a single step of such weighted- $L_1$  regularization is enough to get solutions that are close to optimal, so long as the pre-estimates are *good enough* starting points. The crux of success is finding starts that are, indeed, good enough.

This article provides a complete framework for sparse diminishing-bias regularization that combines ideas from OSE with the concept of a *regularization path* – a general technique, most famously associated with the LARS algorithm (Efron et al., 2004), that estimates a sequence of models under decreasing amounts of regularization. So long as the estimates do not change too quickly along the path, such algorithms can be very fast to run and are an efficient way to obtain a high-quality *set* of models to choose amongst.

A path of one-step estimators (POSE; Algorithm 1) provides  $L_1$  penalized regression on a grid of decreas-

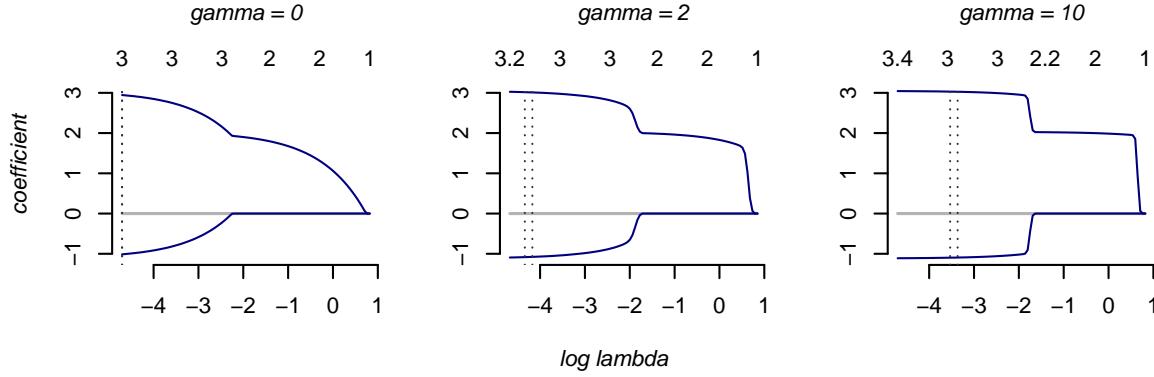


Figure 1: Gamma lasso estimation on  $n = 10^3$  observations of  $y_i = 4 + 3x_{1i} - x_{2i} + \varepsilon_i$ , where  $\varepsilon_i \stackrel{\text{ind}}{\sim} N(0, 1)$  and  $\{x_{1i}, x_{2i}, x_{3i}\}$  are marginally standard normal with correlation of 0.9 between covariates ( $x_{3i}$  is spurious). The penalty path has  $T = 100$  segments,  $\lambda^1 = n^{-1} |\sum_i x_{1i} y_i|$ , and  $\lambda^{100} = 0.01\lambda^1$ . Degrees of freedom are on top and vertical lines mark AICc and BIC selected models (see Section 4).

ing penalties, but adapts coefficient-specific weights to decrease as a function of the coefficient estimated in the previous path step. POSE takes advantage of the natural match between path algorithms and one-step estimation: OSE relies upon inputs being close to the optimal solution, which is precisely the setting where path algorithms are most efficient. We formalize ‘close’ with a novel result in Theorem 3.1 that relates weighted- $L_1$  to  $L_0$  regularization.

This framework allows us to provide

- a *path* of coefficient fits, each element of which corresponds to sparse diminishing-bias regularization estimation under a different level of penalization; where
- obtaining the path of coefficient fits requires no more computation than a state-of-the-art  $L_1$  regularization path algorithm; and
- there are reliable closed-form rules for selection of the optimal penalty level along this path.

The last capability here is derived from a Bayesian interpretation for our *gamma lasso* implementation of POSE from which we are able to construct heuristic information criteria for penalty selection. We view such tools as an essential ingredient for practical applicability in large-scale industrial machine learning where, e.g., cross-validation is not always viable or advisable.

The remainder of this paper is outlined as follows. Section 2 presents the general regularized regression problem and introduces POSE, our path of one-step estimators algorithm, and the gamma lasso (GL), our implemented version of POSE. Section 3 gives an overview on the relationship between concave and weighted- $L_1$  regularization. Section 4 provides a Bayesian model interpretation for the gamma lasso, and derives from this model a set of information criteria that can be applied in penalty selection along the regularization path.

Finally, Section 5 presents two empirical studies: an extensive simulation experiment in 5.1, and in 5.2 we investigate the data analysis question: given all goals in the past decade of NHL hockey, what can we say about individual player contributions?

## 2 Paths of one-step estimators

Denote  $n$  response observations as  $\mathbf{y} = [y_1, \dots, y_n]'$  and the associated matrix of  $p$  covariates as  $\mathbf{X} = [\mathbf{x}_1 \dots \mathbf{x}_n]'$ , with rows  $\mathbf{x}_i = [x_{i1}, \dots, x_{ip}]'$  and columns  $\mathbf{x}_j = [x_{1j}, \dots, x_{nj}]'$ .<sup>1</sup> Write  $\eta_i = \alpha + \mathbf{x}_i' \boldsymbol{\beta}$  as the linear equation for observation  $i$ , and denote with  $l(\alpha, \boldsymbol{\beta}) = l(\boldsymbol{\eta})$  an unregularized objective proportional to the negative log likelihood. For example, in Gaussian (linear) regression,  $l(\boldsymbol{\eta})$  is the sum-of-squares  $0.5 \sum_i (y_i - \eta_i)^2$  and in binomial (logistic) regression,  $l(\boldsymbol{\eta}) = -\sum_i [\eta_i y_i - \log(1 + e^{\eta_i})]$  for  $y_i \in [0, 1]$ . A penalized estimator is the solution to

$$\underset{\alpha, \boldsymbol{\beta}_j \in \mathbb{R}}{\operatorname{argmin}} \left\{ l(\alpha, \boldsymbol{\beta}) + n\lambda \sum_{j=1}^p c(|\beta_j|) \right\}, \quad (1)$$

where  $\lambda > 0$  controls overall penalty magnitude and  $c(\cdot)$  is the coefficient cost function.

A few common cost functions are:  $L_2$   $c(|\beta|) \propto \beta^2$  (ridge, Hoerl and Kennard, 1970),  $L_1$   $c(|\beta|) \propto |\beta|$  (lasso, Tibshirani, 1996), the ‘elastic net’ mixture of  $L_1$  and  $L_2$  (Zou and Hastie, 2005), and the log penalty  $c(|\beta|) \propto \log(1 + \gamma|\beta|)$  (Candes et al., 2008). Those that have a non-differentiable spike at zero (all but ridge) lead to sparse estimators, with some coefficients set to exactly zero. The curvature of the penalty away

<sup>1</sup>Since the size of penalized  $\beta_j$  depends upon the units of  $x_{ij}$ , it is common to scale the coefficient by  $\text{sd}(\mathbf{x}_j)$ , the standard deviation of the  $j^{\text{th}}$  column of  $\mathbf{X}$ ; this is achieved if  $x_{ij}$  is replaced by  $x_{ij}/\text{sd}(\mathbf{x}_j)$  throughout.

from zero dictates then the weight of shrinkage imposed on the nonzero coefficients:  $L_2$  costs increase with coefficient size, lasso's  $L_1$  penalty has zero curvature and imposes constant shrinkage, and as curvature goes towards  $-\infty$  one approaches the  $L_0$  penalty of subset selection. In this article we are primarily interested in *concave cost functions*, like the log penalty, which span the range between  $L_1$  and  $L_0$  penalties.

Penalty size,  $\lambda$ , acts as a *squelch*: it suppresses noise to focus on the true input signal. Large  $\lambda$  lead to very simple model estimates, while as  $\lambda \rightarrow 0$  we approach maximum likelihood estimation (MLE). Since you don't know optimal  $\lambda$ , practical application of penalized estimation requires a *regularization path*: a  $p \times T$  field of  $\hat{\beta}$  estimates, say  $\hat{\beta}|_{\lambda}$ , obtained while moving from high to low penalization along  $\lambda^1 > \lambda^2 \dots > \lambda^T$ . These paths begin at  $\lambda^1$  set to infimum  $\lambda$  such that (1) is minimized at  $\hat{\beta}|_{\lambda} = \mathbf{0}$ , and proceed down to some pre-specified  $\lambda^T$  (e.g.,  $\lambda^T = 0.01\lambda^1$ ).

Our path of one-step estimators (POSE) framework is in Algorithm 1. In this, we are assuming a penalty specification such that  $\lim_{b \rightarrow 0} c'(|b|) = 1$  and that the cost function is differentiable for  $b \neq 0$ .

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#### Algorithm 1 POSE

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Initialize  $\lambda^1 = \inf \{ \lambda : \hat{\beta}|_{\lambda} = \mathbf{0} \}$ , so that  $\hat{\beta}_1 = \mathbf{0}$ .

Set step size  $0 < \delta < 1$ .

for  $t = 2 \dots T$ :

$$\lambda^t = \delta \lambda^{t-1}$$

$$\omega_j^t = \begin{cases} c'(|\hat{\beta}_j^{t-1}|) & \text{for } j \in \hat{S}_t \\ 1 & \text{for } j \in \hat{S}_t^c \end{cases} \quad (2)$$

$$[\hat{\alpha}, \hat{\beta}]^t = \underset{\alpha, \beta_j \in \mathbb{R}}{\operatorname{argmin}} l(\alpha, \beta) + n \sum_j \lambda^t \omega_j^t |\beta_j| \quad (3)$$


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Section 3 will detail how POSE relates to concave regularization. However, for some quick intuition, consider POSE with a concave cost function (such as the log penalty in Figure 2). The derivative  $c'(|\hat{\beta}|)$  will be positive but decreasing with larger values of  $\hat{\beta}$ , such that the *weight* on the  $L_1$  penalty for  $\hat{\beta}_j^t$  will *diminish* with the size of  $|\hat{\beta}_j^t|$ . This implies that coefficient estimates later in the path will be less biased towards zero if that coefficient has a large value earlier in the path.

## 2.1 The gamma lasso

The gamma lasso (GL) specification for POSE is based upon the log penalty,

$$c(\beta_j) = \log(1 + \gamma|\beta_j|), \quad (4)$$

where  $\gamma > 0$ . This penalty is concave with curvature  $-1/(\gamma^{-1} + |\beta_j|)^2$  and it spans the range from  $L_0$  ( $\gamma \rightarrow \infty$ ) to  $L_1$  ( $\gamma \rightarrow 0$ ) costs. It appears under a variety of parameterizations and names in the literature; see Mazumder et al. (2011) and applications in Friedman (2008), Candès et al. (2008), Cevher (2009), Taddy (2013b) and Armagan et al. (2013).

GL simply replaces line (2) in Algorithm 1 with

$$\omega_j^t = \left(1 + \gamma|\hat{\beta}_j^{t-1}|\right)^{-1} \quad j = 1 \dots p \quad (5)$$

Behavior of the resulting paths is governed by  $\gamma$ , which we refer to as the penalty *scale*. Under  $\gamma = 0$ , GL is just the usual lasso. Bias diminishes faster for larger  $\gamma$  and, at the extreme,  $\gamma = \infty$  yields a subset selection routine where a coefficient is unpenalized in all segments after it first becomes nonzero. Figure 1 shows solutions in a simple problem.

Each gamma lasso path segment is solved through coordinate descent (see supplement). The algorithm is implemented in `c` as part of the `gamlr` package for R. Usage of `gamlr` mirrors that of its convex penalty analogue `glmnet` (Friedman et al., 2010), the fantastic and widely used package for costs between  $L_1$  and  $L_2$  norms. In the lasso case ( $\gamma = 0$ ), the two algorithms are essentially equivalent.

## 3 Weighted- $L_1$ approximations to concave penalization

Concave penalties such as the log penalty, which have a gradient that is decreasing with absolute coefficient size, yield the ‘diminishing-bias’ property discussed above. It is *the* reason why one would use concave penalization instead of  $L_1$  or convex alternatives.

Unfortunately, such penalties can overwhelm the convex likelihood and produce a concave minimization objective; see Figure 2. This makes computation difficult. For example, one run of SCAD via the `ncvreg` R package (Breheny and Huang, 2011) for the simulation in Section 5.1 requires around 10 minutes, compared to 1-2 seconds for lasso (or gamma lasso). The most efficient exact solver that we've found is the `sparsenet` of Mazumder et al. (2011), also implemented in R, which first fits a lasso path under decreasing  $L_1$  penalty magnitude and, for each segment on this path, adapts coefficient estimates along a second path of increasing penalty concavity. However, `sparsenet` relies upon solution over a large set of specifications<sup>2</sup> and its compute cost remains much higher than for the [gamma] lasso.

<sup>2</sup>POSE shares with `sparsenet` the idea of moving along a path of closely related specifications, but does not require a grid in both cost size and concavity. Intuitively, POSE runs a path diagonally through this grid.

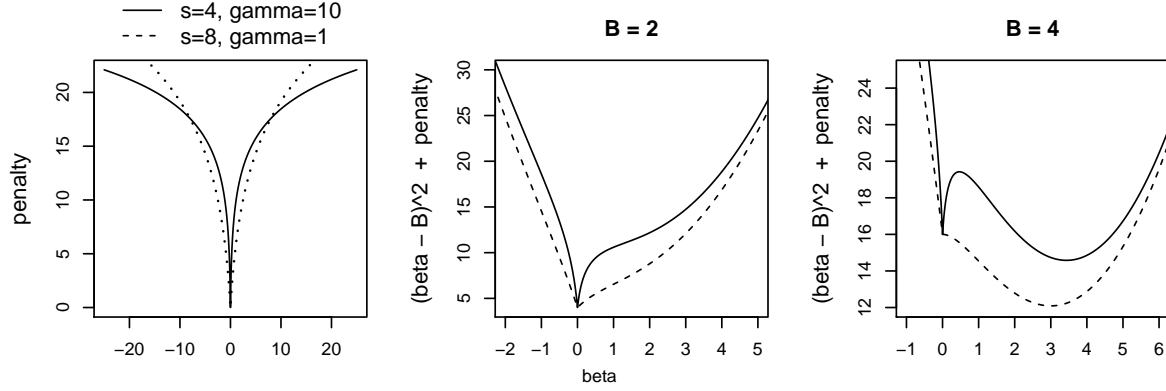


Figure 2: Log penalties  $c(\beta) = s \log(1 + \gamma|\beta|)$  and penalized objectives  $(\beta - B)^2 + c(\beta)$ .

Local linear approximation (LLA; e.g., Candès et al., 2008) algorithms replace the concave cost function  $c$  with its tangent at the current estimate,  $c'(\hat{\beta}_j)\beta_j$ . The objective is then just a weighted  $L_1$  penalized loss. An exact LLA solver iterates between updating  $c'(\hat{\beta})$  and solving the implied  $L_1$  penalized minimization problem. More importantly for POSE, Zou and Li (2008) present numerical and theoretical evidence that LLA can provide near-optimal solutions even (or especially) if you *stop it after one iteration*. This is an example of one-step estimation (OSE), a technique inspired by Bickel (1975) that amounts to taking as your estimator the first step of an iterative approximation to some objective. Such early-stopping can be as good as the full-step solution *if* the initial estimates are good enough.

OSE and similar ideas have had a resurgence in the concave penalization literature recently, motivated by the need for faster estimation algorithms. Fan et al. (2014) consider early-stopping of LLA for folded concave penalization and show that, under strong sparsity assumptions about true  $\beta$  and given appropriate initial values, OSE LLA is with high probability an oracle estimator. Zhang (2010, 2013) investigates ‘convex relaxation’ iterations, where estimates under convex regularization are the basis for weights in a subsequent penalized objective. He shows that just one or two steps here is sufficient for obtaining oracle support recovery properties under much weaker conditions than required by a standard lasso. Wang et al. (2013) propose a two step algorithm that feeds lasso coefficients into a linear approximation to folded concave penalization. These OSE methods are all closely related to the adaptive lasso (AL; Zou, 2006), which does weighted- $L_1$  minimization under weights  $\omega_j = 1/|\hat{\beta}_j^0|$ , where  $\hat{\beta}_j^0$  is an initial guess at the coefficient value. The original AL paper advocates using MLE estimates for initial values, while Huang et al. (2008) suggest using marginal regression coefficients  $\hat{\beta}_j^0 = \text{cor}(\mathbf{x}_j, \mathbf{y})$ .<sup>3</sup>

The main point here is that OSE LLA, or a two-step estimator starting from  $\hat{\beta} = 0$ , or any version of the

adaptive lasso, are all interpretable as weighted- $L_1$  penalization with weights equal to something like  $c'(\beta^0)$  for initial coefficient guess  $\beta^0$ . POSE and GL take advantage of an available source of initial values in any path estimation algorithm – the solved values from the previous path iteration. Our simulations in Section 5.1 show that this efficient strategy works as well or better than expensive exact solvers. In the next section, we provide some theoretical intuition on why it works.

### 3.1 Comparison between weighted- $L_1$ and $L_0$ penalized estimation

Our oracle benchmark is estimation under  $L_0$  costs,  $c(\beta_j) = \mathbb{1}_{\{\beta_j \neq 0\}}$ , for which global solution is impractical. We are interested in weighted- $L_1$  penalization as a way to obtain fits that are as sparse as possible without compromising predictive ability, regardless of the underlying data generating process (or ‘true’ sparsity).

For any support subset  $S \subset \{1 \dots p\}$  with cardinality  $|S| = s$  and complement  $S^c = \{1 \dots p\} \setminus S$ , denote vectors restricted to  $S$  as  $\beta_S = [\beta_j : j \in S]'$ , matrices as  $\mathbf{X}_S$ , etc. Use  $\beta^S$  to denote the coefficients for ordinary least-squares (OLS) restricted to  $S$ : that is,  $\beta_S^S = (\mathbf{X}_S' \mathbf{X}_S)^{-1} \mathbf{X}_S' \mathbf{y}$  and  $\beta_j^S = 0 \forall j \notin S$ . Moreover,  $\mathbf{e}^S = \mathbf{y} - \mathbf{X} \beta^S = (\mathbf{I} - \mathbf{H}^S) \mathbf{y}$  are residuals and  $\mathbf{H}^S = \mathbf{X}_S (\mathbf{X}_S' \mathbf{X}_S)^{-1} \mathbf{X}_S'$  the hat (projection) matrix from OLS restricted to  $S$ .<sup>4</sup>

We use the following result for iterative *stagewise* regression, with proof in the supplemental appendix.

**Lemma 3.1.** Say  $\text{MSE}_S = \|\mathbf{X} \beta^S - \mathbf{y}\|^2/n$  and  $\text{cov}(\mathbf{x}_j, \mathbf{e}^S) = \mathbf{x}_j' (\mathbf{y} - \mathbf{X} \beta^S)/n$  are sample variance and covariances. Then for any  $j \in 1 \dots p$ ,

$$\text{cov}^2(\mathbf{x}_j, \mathbf{e}^S) \leq \text{MSE}_S - \text{MSE}_{S \cup j}$$

In addition, we need to define *restricted eigenvalues* (RE) on the gram matrix  $\mathbf{X}'\mathbf{X}/n$ .<sup>5</sup>

<sup>4</sup>We suppress intercepts throughout, and use  $|\cdot|$  and  $\|\cdot\|$  applied to vectors as the  $L_1$  and  $L_2$  norms, respectively.

<sup>5</sup>This RE matches the ‘adaptive restricted eigenvalues’ of

<sup>3</sup>We include marginal AL in our study of Section 5.1.

**Definition 3.1.** The restricted eigenvalue is  $\phi^2(L, S) = \min_{\{\mathbf{v}: \mathbf{v} \neq \mathbf{0}, |\mathbf{v}_{S^c}| \leq L\sqrt{s}\|\mathbf{v}_S\|\}} \frac{\|\mathbf{X}\mathbf{v}\|^2}{n\|\mathbf{v}\|^2}$ .

Finally, we bound the distance between prediction rules from  $L_0$  and weighted- $L_1$  penalized estimation.

**Theorem 3.1.** Consider squared-error loss  $l(\beta) = \frac{1}{2}\|\mathbf{X}\beta - \mathbf{y}\|^2$ , and suppose  $\beta^\nu$  minimizes the  $L_0$  penalized objective  $l(\beta) + n\nu \sum_{j=1}^p \mathbb{1}_{\{\beta_j \neq 0\}}$  with  $\beta^\nu = \beta^S$  and  $|S| = s < n$ . Write  $\hat{\beta}$  as solution to the weighted- $L_1$  minimization  $l(\beta) + n\lambda \sum_j \omega_j |\beta_j|$ .

Then  $\omega_{S^c}^{\min} \lambda > \sqrt{2\nu}$  while  $\phi^2(L, S) > 0$  implies

$$\frac{\|\mathbf{X}(\hat{\beta} - \beta^\nu)\|^2}{n} \leq \frac{4\lambda^2 \|\omega_S\|^2}{\phi^2(L, S)} \quad (6)$$

with  $L = \frac{\|\omega_S\|}{\sqrt{s}} (\omega_{S^c}^{\min} - \sqrt{2\nu}/\lambda)^{-1}$  for the RE.

*Proof.* From the definitions of  $\hat{\beta}$  and  $\beta^\nu = \beta^S$ ,

$$\begin{aligned} & \frac{1}{2}\|\mathbf{X}\hat{\beta} - \mathbf{y}\|^2 + n\lambda \sum_j \omega_j |\hat{\beta}_j| \\ &= \frac{\|\mathbf{X}(\hat{\beta} - \beta^\nu)\|^2}{2} + \frac{\|\mathbf{e}^S\|^2}{2} - \hat{\mathbf{y}}' \mathbf{e}^S + n\lambda \sum_j \omega_j |\hat{\beta}_j| \\ &\leq \frac{1}{2}\|\mathbf{e}^S\|^2 + n\lambda \sum_{j \in S} \omega_j |\beta_j^S| \end{aligned} \quad (7)$$

Since  $\hat{\mathbf{y}}' \mathbf{e}^S = \hat{\mathbf{y}}'(\mathbf{I} - \mathbf{H}^S)\mathbf{y} = \hat{\beta}' \mathbf{X}'(\mathbf{y} - \mathbf{X}\beta^\nu) = \sum_{j \in S^c} \hat{\beta}_j \mathbf{x}_j'(\mathbf{y} - \mathbf{X}\beta^\nu)$ , we can apply Lemma 3.1 followed by  $\beta^\nu$  being optimal under  $L_0$  penalty  $\nu$  to get

$$\left( \frac{\mathbf{x}_j'(\mathbf{y} - \mathbf{X}\beta^\nu)}{n} \right)^2 \leq \text{MSE}_S - \text{MSE}_{S \cup j} < 2\nu \quad \forall j \quad (8)$$

so that  $|\hat{\mathbf{y}}' \mathbf{e}^S| = |\hat{\beta}_{S^c}' \mathbf{X}'_{S^c}(\mathbf{y} - \mathbf{X}\beta^\nu)| < n\sqrt{2\nu} |\hat{\beta}_{S^c}|$ . Applying this inside (7),

$$\begin{aligned} & \frac{1}{2}\|\mathbf{X}(\hat{\beta} - \beta^\nu)\|^2 + n(\omega_{S^c}^{\min} \lambda - \sqrt{2\nu}) |\hat{\beta}_{S^c}| \\ &\leq n\lambda \sum_{j \in S} \omega_j |\hat{\beta}_j - \beta_j^\nu| \leq n\lambda \|\omega_S\| \|\hat{\beta}_S - \beta_S^\nu\|. \end{aligned} \quad (9)$$

Given  $\omega_{S^c}^{\min} \lambda > \sqrt{2\nu}$ , difference  $\hat{\beta} - \beta^\nu$  is in the RE support for  $L = \frac{\|\omega_S\|}{\sqrt{s}} (\omega_{S^c}^{\min} - \sqrt{2\nu}/\lambda)^{-1}$  and thus  $\|\hat{\beta}_S - \beta_S^\nu\| \leq \|\mathbf{X}(\hat{\beta} - \beta^\nu)/\sqrt{n}\|/\phi(L, S)$ . Finally, applying this inside (9) yields

$$\frac{1}{2}\|\mathbf{X}(\hat{\beta} - \beta^\nu)\|^2 \leq \frac{\sqrt{n}\lambda \|\omega_S\| \|\mathbf{X}(\hat{\beta} - \beta^\nu)\|}{\phi(L, S)}. \quad (10)$$

Dividing each side by  $\sqrt{n}\|\mathbf{X}(\hat{\beta} - \beta^\nu)\|/2$  and squaring gives the result.  $\square$

Buhlmann and van de Geer (2011). Similar quantities are common in the theory of regularized estimators; see also Raskutti et al. (2010) and Bickel et al. (2009).

## Remarks

- Theorem 3.1 is finite sample exact. Distinguishing it from related results in the literature, it is also completely *non-parametric* – it makes no reference to the true distribution of  $\mathbf{y}|\mathbf{X}$ . Indeed, if we make such assumptions, Theorem 3.1 provides bounds on the distance between a weighted-lasso and optimal prediction. The next remark is an example.

- Assume that  $\mathbf{y} \sim (\boldsymbol{\eta}, \sigma^2 \mathbf{I}) - y_i$  independent with mean  $\mu_i$  and shared variance  $\sigma^2$ . The  $C_p$  formula of Mallows (1973) gives  $\text{MSE}_S + 2s\sigma^2/n$  as an unbiased estimate of residual variance. Following Efron (2004), this implies  $\nu = \sigma^2/n$  is the optimal  $L_0$  penalty for minimizing prediction error. Theorem (3.1) applies directly, with  $L = \frac{\|\omega_S\|}{\sqrt{s}} (\omega_{S^c}^{\min} - \sqrt{2\sigma^2}/(\lambda\sqrt{n}))^{-1}$ , to give a bound on the distance between weighted- $L_1$  estimation and  $C_p$ -optimal prediction.<sup>6</sup> Note that, since the condition on minimum  $S^c$  weights has become  $\omega_{S^c}^{\min} > (\sigma/\lambda)\sqrt{2/n}$ , comparison to  $C_p$  suggests we can use larger  $\gamma$  with large  $n$  or small  $\sigma$ .

- Plausibility of the restricted eigenvalue assumption  $\phi(L, S) > 0$  depends upon  $L$ . It is less restrictive if we can reduce  $\|\omega_S\|$  without making  $\omega_{S^c}^{\min}$  small. *This is a key motivation for the POSE algorithm:* if covariates with nonzero  $\hat{\beta}_j$  for large  $\lambda$  (i.e., early in the path) can be assumed to live in  $S$ , then increasing  $\gamma > 0$  will improve prediction. Of course, the moment that  $\lambda$  becomes small enough that elements of  $S^c$  get nonzero  $\hat{\beta}$ , then larger  $\gamma$  can lead to over-fit. For this reason it is essential that we have tools for choosing optimal  $\lambda$ .

- In the supplemental material, we also adapt standard results from Wainwright (2006, 2009) to show how reducing  $\|\omega_S\|$  without making  $\omega_{S^c}^{\min}$  small can lead to lower false discovery rates with respect to the  $L_0$  oracle. However, such results depend upon design restrictions that are less realistic in practice.

## 4 Penalty selection

### 4.1 Bayesian motivation

Consider a model where each  $\beta_j$  is assigned a Laplace distribution prior with scale  $\tau_j > 0$ ,

$$\beta_j \sim \text{La}(\tau_j) = \frac{\tau_j}{2} \exp[-\tau_j |\beta_j|]. \quad (11)$$

Typically, scale parameters  $\tau_1 = \dots = \tau_p$  are set as a single shared value, say  $n\lambda/\phi$  where  $\phi$  is the exponential family dispersion (e.g. Gaussian variance  $\sigma^2$  or 1 for the binomial). Posterior maximization under the prior in (11) is then lasso estimation (e.g., Park and Casella, 2008).

<sup>6</sup>We work with  $C_p$  here, rather than  $AIC$  or  $AIC_c$ , since  $C_p$  is conveniently defined the scale of squared errors.

Instead of working from shared scale, assume an independent gamma  $\text{Ga}(s, 1/\gamma)$  hyperprior with ‘shape’  $s$  and ‘scale’  $\gamma$  for each  $\tau_j$ , such that  $\mathbb{E}[\tau_j] = s\gamma$  and  $\text{var}(\tau_j) = s\gamma^2$ . Then the *joint* prior for both coefficient and scale is

$$\pi(\beta_j, \tau_j) = \text{La}(\beta_j; \tau_j) \text{Ga}(\tau_j; s, \gamma^{-1}) = \frac{1}{2\Gamma(s)} \left( \frac{\tau_j}{\gamma} \right)^s \exp[-\tau_j(\gamma^{-1} + |\beta_j|)] \quad (12)$$

The gamma hyperprior is conjugate here, implying a  $\text{Ga}(s+1, 1/\gamma + |\beta_j|)$  posterior for  $\tau_j \mid \beta_j$  with conditional posterior mode (MAP) at  $\hat{\tau}_j = \gamma s / (1 + \gamma |\beta_j|)$ .

Consider joint MAP estimation of  $[\boldsymbol{\tau}, \boldsymbol{\beta}]$  under the prior in (12), where we’ve suppressed  $\alpha$  for simplicity. By taking negative logs and removing constants, this is equivalent to solving

$$\min_{\beta_j \in \mathbb{R}, \tau_j \in \mathbb{R}^+} \phi^{-1} l(\boldsymbol{\beta}) + \sum_j [\tau_j(\gamma^{-1} + |\beta_j|) - s \log(\tau_j)] \quad (13)$$

It is straightforward to show that (13) is equivalent to the log-penalized objective

$$\min_{\beta_j \in \mathbb{R}} \phi^{-1} l(\boldsymbol{\beta}) + \sum_j s \log(1 + \gamma |\beta_j|) \quad (14)$$

**Proposition 4.1.**  $\hat{\boldsymbol{\beta}}$  solves (14) if and only if it is also in the solution to (13).

*Proof.* The conditional posterior mode for each  $\tau_j$  given  $\beta_j$  is  $\tau(\beta_j) = \gamma s / (1 + \gamma |\beta_j|)$ . Any joint solution  $[\hat{\boldsymbol{\beta}}, \hat{\boldsymbol{\tau}}]$  for (13) thus consists of  $\hat{\tau}_j = \tau(\hat{\beta}_j)$ ; otherwise, it is always possible to decrease the objective by replacing  $\hat{\tau}_j$ . Setting each  $\tau_j = \tau(\beta_j)$  in (13) and removing constant terms yields (14). Moreover, the solution to (13) solves (14): otherwise, there would need to be a point on the profile slice of (13) defined by  $\tau_j = \tau(\hat{\beta}_j)$  that is lower than its minimum.  $\square$

For a Bayesian it is odd to be solving for  $\boldsymbol{\tau}$  rather than marginalizing over its uncertainty. However, recognizing the form of a gamma density in (12),  $\pi(\beta_j, \tau_j)$  integrates over  $\tau_j$  to yield the marginal prior  $\pi(\beta_j) = 0.5s(1 + \gamma |\beta_j|)^{-(s+1)}$ . This is the generalized double Pareto density, as in Armagan et al. (2013). Since  $-\log \pi(\beta_j) \propto (s+1) \log(1 + \gamma |\beta_j|)$ , the *profile* MAP solution to (13) is also the *marginal* MAP for  $\boldsymbol{\beta}$  under  $\text{Ga}(s-1, 1/\gamma)$  priors on each  $\tau_j$ .

## 5 Examples

### 5.1 Simulation

This section will analyze data simulated from the following  $p = 1000$  dimensional regression.

$$y \sim \text{N}(\mathbf{x}'\boldsymbol{\beta}, \sigma^2) \quad \text{where } \mathbf{x} = \mathbf{u} * \mathbf{z}, \quad \mathbf{u} \sim \text{N}(\mathbf{0}, \boldsymbol{\Sigma}), \quad z_j \stackrel{\text{ind}}{\sim} \text{Bin}(0.5), \quad \beta_j = \exp[-\tau_j(\gamma^{-1} + |\beta_j|)] \quad (15)$$

Each simulation draws  $n = 1000$  means  $\eta_i = \mathbf{x}_i'\boldsymbol{\beta}$ , and two independent response samples  $\mathbf{y}, \tilde{\mathbf{y}} \sim \text{N}(\boldsymbol{\eta}, \sigma^2 \mathbf{I})$ . Residual variance  $\sigma^2$  and covariate correlation  $\boldsymbol{\Sigma}$  are adjusted across runs. In the first case, we define  $\sigma^2$  through *signal-to-noise* ratios  $\text{sd}(\boldsymbol{\eta})/\sigma$  of 1/2, 1, and 2. In the latter case, multicollinearity is parametrized via  $\Sigma_{jk} = \rho^{|j-k|}$ , and we consider  $\rho = 0, 0.5$ , and 0.9.

The regression in (15) is obviously *dense*: true coefficients are all nonzero. However, they decay in magnitude along the index  $j$  and it will be useless to estimate many of them in a  $p = n$  regression. Our sparse oracle comparator is the  $C_p$  optimal  $L_0$  penalized solution

$$\boldsymbol{\beta}^* = \underset{\boldsymbol{\beta}}{\text{argmin}} \left\{ \|\mathbf{y} - \mathbf{X}\boldsymbol{\beta}\|^2 + 2\sigma^2 \sum_j \mathbb{1}_{\{\beta_j \neq 0\}} \right\}, \quad (16)$$

which is solvable here by searching through OLS regression on  $\mathbf{X}_{\{1 \dots j\}}$  for  $j = 1 \dots p$ .

We consider `gamlr` runs of GL with  $\gamma$  of 0 (lasso), 2, and 10 and marginal AL, as well as `sparsenet`’s MCP penalized regression. Covariate penalties are standardized by  $\text{sd}(\mathbf{x}_j)$ , and paths run through 100  $\lambda$  values down to  $\lambda^{100} = 0.01\lambda^1$ . On an Intel Xeon E5-2670 core, 5-fold CV with  $\text{sd}(\boldsymbol{\eta})/\sigma = 1$  and  $\rho = 1/2$  requires 1-2 seconds for lasso and marginal AL, 2 and 3 seconds for GL with  $\gamma = 2$  and  $\gamma = 10$ , and 15-20 seconds for `Sparsenet`.<sup>7</sup>

Figures 3 and 4 illustrate GL paths for a single dataset, with  $\text{sd}(\boldsymbol{\eta})/\sigma = 1$  and  $\rho = 1/2$ . In Figure 3, increasing  $\gamma$  leads to ‘larger shouldered’ paths where estimates move quickly to MLE for the nonzero-coefficients. Degrees of freedom, calculated as in (??), are along the top of each plot; equal  $\lambda$  have higher  $df^t$  for higher  $\gamma$  since there is less shrinkage of  $\hat{\beta}_j \neq 0$ . Figure 4 shows CV and AICc error estimates. The two criteria roughly track each other, although AICc more heavily penalizes over-fit and at  $\gamma = 10$  their minima do not match. Notice that as  $\gamma$  increases, the CV error

<sup>7</sup>`ncvreg` SCAD required ten minutes for a single run and is thus impractical for the applications under consideration. But, in a small study, CV.min selected SCAD performs quite well in prediction – similarly to the best CV.min methods for each data configuration – with relatively high values for both false discovery and sensitivity.

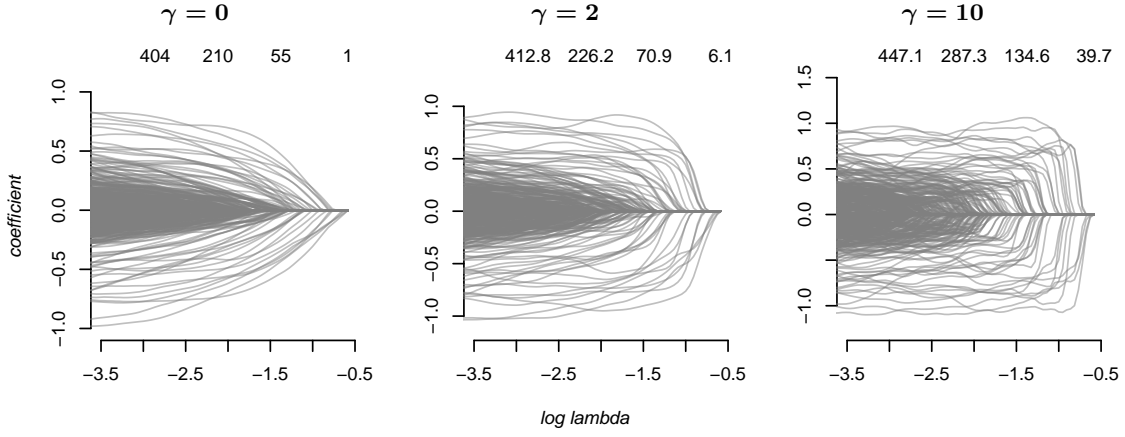


Figure 3: Regularization paths for simulation example. Degrees of freedom  $df^t$  are along the top.

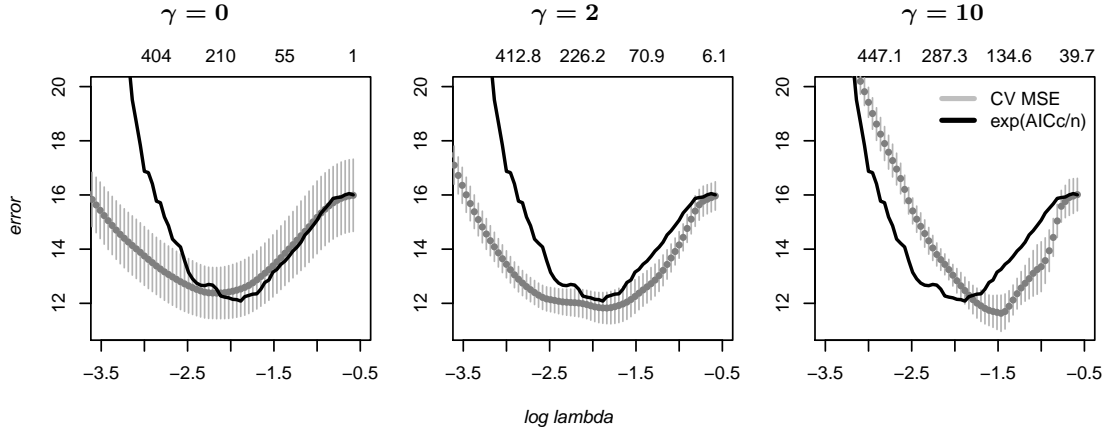


Figure 4: 5-fold CV and AICc for a simulation example. Points-and-bars show mean OOS MSE  $\pm 1se$ .

increases more quickly after it's minimum; this indicates that the consequences of over-fit are worse under faster diminishing-bias.

## 5.2 Hockey players

This section attempts to quantify the performance of hockey players. It extends analysis in Gramacy et al. (2013). The current version includes data about who was on the ice for every goal in the National Hockey League (NHL) back to the 2002-2003 season, including playoffs. The data are in the `gamlr` package; there are 69449 goals and 2439 players.

The logistic regression model of player contribution is, for goal  $i$  in season  $s$  with away team  $a$  and home team  $h$ ,

$$\text{logit}[p(\text{home team scored goal } i)] = \alpha_0 + \alpha_{sh} - \alpha_{sa} + \mathbf{u}_i \boldsymbol{\beta}_0 + \mathbf{x}_{i0} \boldsymbol{\beta}_0 + \mathbf{x}_{is} \boldsymbol{\beta}_s, \quad (17)$$

Vector  $\mathbf{u}_i$  holds indicators for various special-teams scenarios (e.g., a home team power play), and  $\boldsymbol{\alpha}$  provides matchup/season specific intercepts. Vector  $\mathbf{x}_i$  contains player effects:  $x_{ij} = 1$  if player  $j$  was on the

home team and on ice for goal  $i$ ,  $x_{ij} = -1$  for away player  $j$  on ice for goal  $i$ , and  $x_{ij} = 0$  for everyone not on the ice. Coefficient  $\beta_{0j} + \beta_{sj}$  is the season- $s$  effect of player  $j$  on the log odds that, given a goal has been scored, the goal was scored by their team. These effects are ‘partial’ in that they control for who else was on the ice, special teams scenarios, and team-season fixed effects – a player’s  $\beta_{0j}$  or  $\beta_{sj}$  only need be nonzero if that player effects play above or below the team average for a given season.

We estimate gamma lasso paths of  $\boldsymbol{\beta}$  for the model in (17) with  $\boldsymbol{\alpha}$  and  $\boldsymbol{\phi}$  left unpenalized. In contrast to the default for most analyses, our coefficient costs are *not* scaled by covariate standard deviation. Doing the usual standardization would have favored players with little ice time. The algorithm is run for  $\log_{10} \gamma = -5 \dots 2$ , plus the  $\gamma = 0$  lasso.<sup>8</sup>

Joint  $[\boldsymbol{\alpha}, \boldsymbol{\beta}]$  surfaces for AICc and BIC are in Figure 5. AICc favors denser models with low  $\lambda$  but not-to-big  $\gamma$ , while the BIC prefers very sparse but relatively unbiased models with large  $\lambda$  and small  $\gamma$ . Both criteria

<sup>8</sup>On this data,  $\gamma = \infty$  subset selection yields perfect separation and infinite likelihood.

are strongly adverse to any model at  $\gamma = 100$ , which is where timings explode in Figure ???. Ten-fold CV results are shown in Figure 6 for  $\gamma$  of 0, 1, and 10. The OOS error minima are around the same in each case – average deviance slightly above 1.16 – but errors increase much faster away from optimality with larger  $\gamma$ . We also see that AICc selection is always between the CV.min and CV.lse selections: at  $\gamma = 0$  AICc matches the CV.lse choice, while at  $\gamma = 10$  it has moved right to the CV.lse selection. Our heuristic from Section ???.2 might be over-estimating  $df$  for large- $\gamma$  models (especially under this very collinear design), but one would also suspect that CV estimates of minimum deviance are biased downward more dramatically for larger  $\gamma$  than for low-variance small- $\gamma$  estimators.

The motivating application for this example was to devise a better versions of hockey’s ‘plus-minus’ (PM) statistic: number of goals *for* minus *against* each player’s team while he is on the ice. To convert from player effects  $\beta_{0j} + \beta_{sj}$  to the scale of ‘plus/minus’, we first state that in absence of any other relevant information about each goal (not team, home/away, etc), the probability a goal was scored by his team given player  $j$  is on ice becomes  $p_j = e^{\beta_j} / (1 + e^{\beta_j})$  and our ‘partial plus/minus’ (PPM) is

$$\text{ppm}_j = N_j(p_j - (1 - p_j)) = N_j(2p_j - 1)$$

where  $N_j$  is the number of goals for which he was on-ice. This measures quality and quantity of contribution, controlling for confounding information, and lives on the same scale as PM.

Table 1 contains the estimated PPM values for the 2013-2014 season under various  $\gamma$  levels, using AICc selection. We see that, even if changing concavity ( $\gamma$ ) has little effect on minimum CV errors, larger  $\gamma$  yield more sparse models and different conclusions about player contribution. At the  $\gamma = 0$  lasso, there are 305 nonzero player effects (individuals measurably different from their team’s average ability) and the list includes young players who have had very strong starts to their careers. For example, Ondrej Palat and Tyler Toffoli both played their first full seasons in the NHL in 2013-2014. As  $\gamma$  increases to 1, these young guys drop in rank while more proven stars (e.g., Sidney Crosby and Jonathan Toews) move up the list. Finally, at  $\gamma = 10$  only big-name stars remain amongst the 64 nonzero player effects.

## 6 Discussion

Concave penalized estimation in Big data, where exact solvers are too computationally expensive, reduces largely to weighted- $L_1$  penalization. This review has covered a number of topics that we think relevant for

such schemes. Apart from the simulation study, we have not provided extensive comparison of the many available weighting mechanisms. However, we feel that path adaptation is an intuitively reasonable source of weights. In any case, POSE has the advantage that using a regularization path to supply penalty weights is computationally efficient. To scale for truly Big data,  $L_1$  weights need be constructed at practically no cost on top of a standard lasso run. Beyond `gamlr` and marginal regression adaptive lasso, we have found no other software for sparse diminishing bias estimation where this standard is met.

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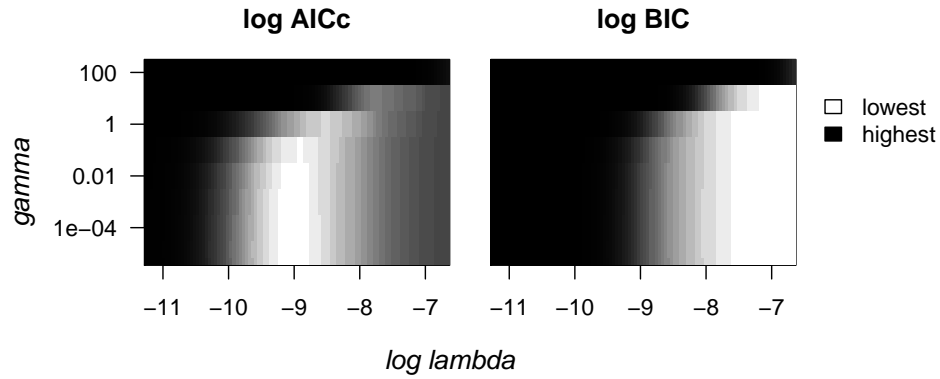


Figure 5: Hockey example AICc and BIC surfaces, rising from white to black on log scale.

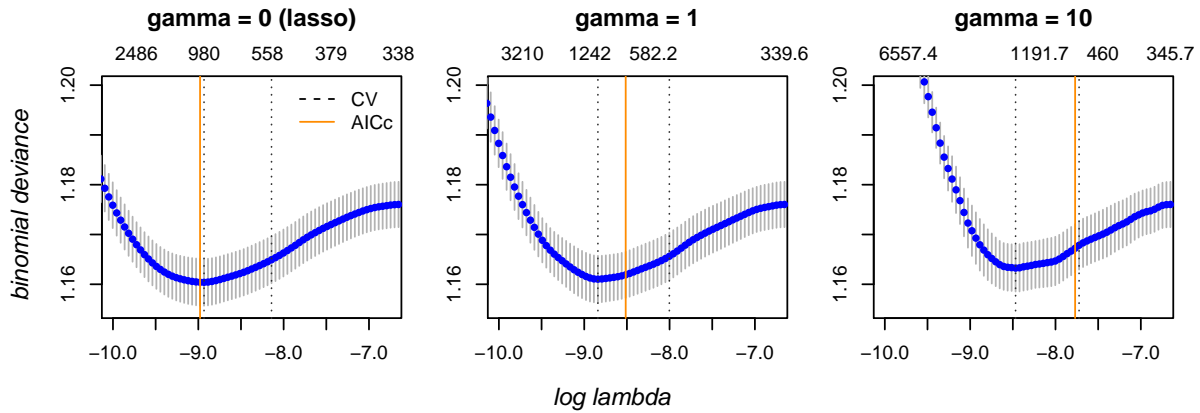


Figure 6: Hockey example 10-fold CV: mean OOS deviance  $\pm 1se$ , with minimum-error and 1SE selection rules marked with black dotted lines, and solid orange line showing AICc selection.

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<i>lasso</i>		$\gamma = 1$		$\gamma = 10$		
		PPM	PM	PPM	PM	
1	Ondrej Palat	33.8	38	Sidney Crosby	29.2	52
2	Sidney Crosby	31.2	52	Ondrej Palat	29	38
3	Henrik Lundqvist	25.8	9	Jonathan Toews	21.4	35
4	Jonathan Toews	24	35	Joe Thornton	21	34
5	Andrei Markov	23.1	34	Andrei Markov	20.9	34
6	Joe Thornton	21.4	34	Henrik Lundqvist	19.8	9
7	Anze Kopitar	20.6	39	Anze Kopitar	19.5	39
8	Tyler Toffoli	18.9	31	Pavel Datsyuk	16.1	13
9	Pavel Datsyuk	17.7	13	Logan Couture	15.9	29
10	Ryan Nugent-hopkins	17.4	18	Alex Ovechkin	15.8	16
11	Gabriel Landeskog	16.6	36	Marian Hossa	14.4	21
12	Logan Couture	16.5	29	Alexander Semin	14.2	-1
13	Alex Ovechkin	15.8	16	Matt Moulson	13.9	22
14	Marian Hossa	15.4	21	Tyler Toffoli	13.3	31
15	Alexander Semin	14.8	-1	David Perron	12.7	2
16	Zach Parise	14.7	21	Mikko Koivu	12.5	12
17	Frans Nielsen	13.5	8	Frans Nielsen	12.3	8
18	Mikko Koivu	13.4	12	Ryan Getzlaf	12.1	16
19	Matt Moulson	13.4	22	Ryan Nugent-hopkins	11.9	18
20	David Perron	13.1	2	Jaromir Jagr	11.8	28
<i>305 nonzero effects</i>				<i>204 nonzero effects</i>		
				<i>64 nonzero effects</i>		

Table 1: Top 20 AICc selected player ‘partial plus-minus’ (PPM) values for the 2013-2014 season, under  $\gamma = 0, 1, 10$ . The number of nonzero player effects for each  $\gamma$  are noted along the bottom.

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