Model Selection and Estimation in High-dimensional Generalized Linear Models

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December 7, 2018

1 Introduction

The workhorse for high-dimensional regressions is the ℓ_1 lasso penalty (Tibshirani, 1996). The original lasso is developed for fitting (normal) linear models with the objective[1]

$$\widehat{\boldsymbol{\beta}}_{\text{lasso}} = \arg\min_{\boldsymbol{\beta}} \ \|\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta}\|^2 + \lambda \|\boldsymbol{\beta}\|_1 - \lambda|\beta_0|, \ \lambda > 0. \tag{1}$$

The first paper about lasso in a GLM setting is Park and Hastie (2007): Consider a scalar GLM with likelihood

$$L(y; \theta, \phi) = \exp\left\{\frac{y\theta - b(\theta)}{a(\phi)} + c(y, \phi)\right\},$$

where $g(\mathbb{E}[y]) = \eta = \boldsymbol{x}^\mathsf{T}\boldsymbol{\beta}$ for some scalar function g. Thus we may consider a direct extension of (1):

$$\widehat{\boldsymbol{\beta}}_{\text{GLM-lasso}} = \arg\min_{\boldsymbol{\beta}} \ \underbrace{-\frac{1}{n}\sum_{i=1}^{n}\left[y_i\theta(\boldsymbol{\beta})_i - b\left(\theta(\boldsymbol{\beta})_i\right)\right]}_{\ell_n(\boldsymbol{\beta})} + \lambda\|\boldsymbol{\beta}\|_1 - \lambda|\beta_0|, \tag{2}$$

where (2) reduces to (1) if the likelihood is Gaussian and g is the canonical link for the Gaussian model, which is the identity function. Note that the objective (2) is convex if

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[1]We consider $\boldsymbol{y}$ an n-vector of response variables whose ith element is $\boldsymbol{y}_i$. We consider the covariate matrix $\boldsymbol{X}$ ($n \times p$). In most settings, $\boldsymbol{X}$ include an intercept column, $\boldsymbol{x}_0 = \boldsymbol{1}$, that is not regularized.

we use the canonical link, since the exponential family log-likelihood is concave in θ, and $\theta = \boldsymbol{x}^\intercal \boldsymbol{\beta}$ is linear in $\boldsymbol{\beta}$ for the canonical link.

2 Model Selection with Lasso

Brute-force model selection scales poorly with respect to the number of predictors, yet model selection is most important precisely when we have a large number of predictors. That is, when building a model to predict $\boldsymbol{y}$ from a subset of the columns of $\boldsymbol{X} \in \mathbb{R}^{n,p}$ (since not all columns may be predictive), there are 2^p subsets of columns to regress on. Checking all of these models against each other incurs a cost exponential in p and becomes prohibitively expensive in a high-dimensional setting.

In class, we tackled this problem with forward-selection and backward-deletion, a greedy algorithm that adds and removes covariates until a local optimal is reached. Park and Hastie (2007)'s use of the lasso for GLMs provides a competitive alternative that behaves less greedily. We describe their procedure in this section.

In order to employ this method, we require a method to solve (2). For now, we suppose that we have such a method and can use it as a black box. It is sufficient for us to know that this black box takes in an initial $\boldsymbol{\beta}^{\text{init}}$ and employs a descent-based method to converge toward the optimal $\boldsymbol{\beta}^*$. Section 3 follows-up by describing the inner workings of different approaches.

The lasso penalty induces a sparsity in our optimal $\boldsymbol{\beta}$. This sparsity increases as our penalization term λ becomes bigger. Indeed, if we take $\lambda \to \infty$, then our solution is driven to $\boldsymbol{\beta} \to \boldsymbol{0}$ because the penalization term is all that matters, and the norm of $\boldsymbol{\beta}$ is minimized at $\boldsymbol{0}$. The entire domain when $\boldsymbol{\beta} = \boldsymbol{0}$ is uninteresting, so we initialize our algorithm at $\lambda_{\max}$ which we define as the smallest λ such that there is only one non-zero coefficient.

3 Estimation

Efron et al. (2004) gives an efficient estimation procedure for the linear lasso (1) called the Least Angle Regression (LAR), which relies on the fact that the *regularization path*—$\widehat{\boldsymbol{\beta}}_i$ as a function of λ—is piecewise linear in (1). Such a structure is often unavailable in applications like (2). The most popular method—proposed by Friedman, Hastie, and Tibshirani (2010) and implemented in R's glmnet package—is *cyclical coordinate descent* with iteratively reweighted least squares. The idea is to approximate $\ell_n(\boldsymbol{\beta})$ in (2) with a second-order Taylor expansion, either globally for all parameters $\boldsymbol{\beta}$ (for scalar-valued GLMs) or locally with a single parameter $\boldsymbol{\beta}_j$ (for vector-valued GLMs, such as the multinomial logistic regression). Such an approximation yields a quadratic function (in the scalar GLM case)

$$\ell_Q(\boldsymbol{\beta}) = \frac{1}{n} \sum_{i=1}^{n} w_i (y_i - \boldsymbol{x}_i^{\mathsf{T}} \boldsymbol{\beta})^2.$$

We then solve a local penalized least-squares problem:

$$\boldsymbol{\beta} \leftarrow \arg\min_{\boldsymbol{\beta}} \ell_Q(\boldsymbol{\beta}) + \lambda \left\| \boldsymbol{\beta} \right\|_1. \tag{3}$$

via cyclical coordinate descent, i.e. by iteratively solving

$$\boldsymbol{\beta}_j \leftarrow \arg\min_{\boldsymbol{\beta}_j} \ell_Q(\boldsymbol{\beta}) + \lambda \left\| \boldsymbol{\beta} \right\|_1, \tag{4}$$

holding all other entries $\boldsymbol{\beta}_{-j}$ fixed. (4) has an analytical solution for the lasso penalty[2]

$$\boldsymbol{\beta}_j \leftarrow \frac{S\left(\sum_{i=1}^{N} w_i x_{ij} \left(y_i - \tilde{y}_i^{(j)} \right), \lambda \right)}{\sum_{i=1}^{N} w_i x_{ij}^2}, \ S(t, \gamma) = \text{sgn}(t) \left(|z| - \gamma \right)_+, \ \tilde{y}_i^{(j)} = \boldsymbol{x}_i^{\mathsf{T}} \boldsymbol{\beta} - x_{ij} \boldsymbol{\beta}_j. \tag{5}$$

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[2]Friedman, Hastie, and Tibshirani (2010) show a similar expression for the *elastic net* penalty:

$$\lambda P_\alpha(\boldsymbol{\beta}) = \lambda \left(\alpha \left\| \boldsymbol{\beta} \right\|_1 + (1 - \alpha) \left\| \boldsymbol{\beta} \right\|_2 \right).$$

We summarize the procedure described above in Algorithm 1.

Algorithm 1 Cyclic coordinate descent algorithm for solving (2) (scalar GLM case) in Friedman, Hastie, and Tibshirani (2010)

Initialize $\boldsymbol{\beta}$
for λ on regularization path **do**
    while $\boldsymbol{\beta}$ has not converged **do**
        Approximate $\ell_n(\beta)$ by $\ell_Q(\beta)$
        while cyclical descent has not converged **do**
            for j **do**
                Update $\boldsymbol{\beta}_j$ according to (5)
            end for
        end while
    end while
    $\widehat{\boldsymbol{\beta}}_\lambda \leftarrow \boldsymbol{\beta}$
    Initialize $\boldsymbol{\beta}$ for next iteration to $\widehat{\boldsymbol{\beta}}_\lambda$
end for

The machine learning literature slightly alters Algorithm 1 and changes (5) into

$$\boldsymbol{\beta}_j \leftarrow S\left(\boldsymbol{\beta}_j - (\nabla_{\boldsymbol{\beta}}\ell_n(\boldsymbol{\beta}))_j \, \kappa^{-1}, \frac{\lambda}{\kappa}\right)$$

for some *learning rate* $1/\kappa$, in keeping with gradient descent. Moreover, Shalev-Shwartz and Tewari (2011) proves a convergence guarantee for stochastic coordinate descent in this fashion, where, instead of cycling through the coordinates of $\boldsymbol{\beta}$, a coordinate is chosen uniformly at random.

Theorem 1. Let $Q(\boldsymbol{\beta})$ be the objective in (2). At iteration T of the first while-loop in a verison of Algorithm 1 with stochastic coordinate descent and gradient updates,

$$\mathbb{E}[Q(\boldsymbol{\beta}_T)] - \mathbb{E}[Q(\widehat{\boldsymbol{\beta}}_{\text{GLM-lasso}})] \leq C\frac{p\kappa}{T+1}$$

for constant C a function of the initial starting value $\boldsymbol{\beta}^{(0)}$, assuming that ℓ_n is differentiable with

$$\ell_n(\boldsymbol{\beta} + \eta\boldsymbol{e}_j) \leq \ell_n(\boldsymbol{\beta}) + \eta\left(\nabla\ell_n\right)_j + \frac{\kappa}{2}\eta^2$$

for all $\eta, \boldsymbol{\beta}, j$.[3]

Corollary 2. The runtime to achieve ϵ expected accuracy is bounded by

$$O\left(\frac{np\kappa}{\epsilon} \left\|\widehat{\boldsymbol{\beta}}_{\text{GLM-lasso}}\right\|_2^2\right).$$

Moreover, Bradley et al. (2011) show that a parallel version of the coordinate gradient descent procedure above where at each iteration, P (possibly duplicate) coordinates are updated in parallel. For correlated features, such parallelism is dangerous, since updating two correlated features simulataneously may over or undercompensate for the gradient direction. Bradley et al. (2011) quantifies the interference due to correlated features and shows that efficiency increases linearly in the number of parallel processes P so long as $\mathsf{P} \leq \frac{p}{\rho}$ where ρ is the largest modulus of the eigenvalues of $X^\intercal X$.

Coordinate descent methods described above can also become expensive if n is large. The standard machine learning and optimization answer to this problem is to use *stochastic gradient descent*, replacing $\nabla_{\boldsymbol{\beta}} \ell_n(\boldsymbol{\beta})$ with an unbiased estimate $\boldsymbol{g}_i = \nabla_{\boldsymbol{\beta}} \log L(y_i; \boldsymbol{\beta})$, which is the gradient evaluated on a single observation.[4] Shalev-Shwartz and Tewari (2011) consider a mirror descent algorithm in the lasso context, by running stochastic gradient descent on the dual problem and enforcing sparsity in an intelligent manner. Let $\boldsymbol{\gamma} = f(\boldsymbol{\beta})$ be the dual parameter for $\boldsymbol{\beta}$ with an invertible link f. We choose an observation i at random, compute $\boldsymbol{g}_i$, and update

$$\boldsymbol{\gamma} \leftarrow \boldsymbol{\gamma} - \eta \boldsymbol{g}_i$$

$$\boldsymbol{\gamma}' \leftarrow \boldsymbol{\gamma} - \eta\lambda \operatorname{sgn}(\boldsymbol{\gamma}) \qquad\qquad (\text{Decrease } \|\boldsymbol{\beta}\|_1)$$

$$\gamma_j \leftarrow \gamma_j' \mathbb{1}\left(\operatorname{sgn}(\gamma_j) = \operatorname{sgn}(\gamma_j')\right) \qquad\qquad (\text{Maintains sparsity})$$

$$\boldsymbol{\beta} \leftarrow f^{-1}(\boldsymbol{\gamma}).$$

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[3]This condition restricts the choice of κ as a function of the loss criterion.

[4]We can replace this with *batched gradient descent* as well, where the gradient estimate is averaging over a batch of observations.

The runtime bound for the stochastic mirror descent algorithm in Shalev-Shwartz and Tewari
(2011) is

$$O \left(\frac{p \log p}{\epsilon^2} \left\| \widehat{\boldsymbol{\beta}}_{\text{GLM-lasso}} \right\|_2^2 \right).$$

We pay the price of the $p \log p$ and ϵ^{-2} dependence, as opposed to p and ϵ^{-1}, in order to
achieve the benefit of a n-free runtime.

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