

Bayesian $\sqrt{\text{Lasso}}$

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1 Introduction

Regularized methods have become widely popular as a inferential tool in high-dimensional data, owing to the popularity of Lasso [Tibshirani, 1996] and many of its variants [Tibshirani, 2014]. Regularized methods prevent overfitting by controlling the bias-variance trade-off and are particularly useful for sparse learning, when the number of variables (p) exceed the number of observations (n). In the context of linear regression $Y = X\beta + \epsilon$, a regularized estimate of β is obtained by minimizing the penalized likelihood:

$$\hat{\beta}_{\lambda^*}^{\text{pen}} = \underset{\beta \in \mathbb{R}^p}{\operatorname{argmin}} \{ \|Y - X\beta\|^2 + \lambda^* \Omega(\beta) \}, \quad (1)$$

$$\text{where, } \Omega(\beta) = \sum_{j=1}^p \omega(\beta_j) \text{ is a separable penalty} \quad (2)$$

The gold-standard for regularized method is Lasso that simultaneously performs estimation and model selection by constraining the ℓ_1 norm of the underlying parameter vector, i.e. $\omega(\beta_j) = |\beta_j|$.

$$\hat{\beta}_{\lambda^*}^{\text{lasso}} = \underset{\beta \in \mathbb{R}^p}{\operatorname{argmin}} \{ \|Y - X\beta\|^2 + \lambda^* \|\beta\|_1 \} \quad (3)$$

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Lasso enjoys both computational efficiency, due to LARS [Efron et al., 2004] and coordinate descent [Friedman et al., 2007], as well as theoretical optimality properties [Bühlmann and van de Geer, 2011]. Bickel et al. [2009] have shown that the Lasso estimator achieves near-oracle property in recovering the true β_0 , under Gaussianity and certain design matrix conditions, up to a factor of $\sqrt{\log(2p)}$: yielding a $\sqrt{\log n}$ rate when p grown polynomially as n . However, Lasso's performance in high-dimensional data is critically dependent on estimating the standard deviation σ of the noise ϵ , which remains a non-trivial problem in $p \gg n$ situation. The square-root Lasso, proposed by Belloni et al. [2011], is a modification of Lasso that eliminates the need for knowing σ , or pre-estimating it. The square-root Lasso is also independent of the Gaussianity or sub-gaussianity of noise. In fact, as Giraud [2014] points out, the Lasso estimate with ℓ_1 penalty is not scale-invariant in the sense that the invariance relation $\hat{\beta}(\sigma Y, X) = \sigma \hat{\beta}(Y, X)$ does not hold for all $\sigma > 0$. Since the standard deviation of noise ϵ is σ , one way of obtaining a scale-invariant penalized estimator is to set $\lambda^* = \lambda \sigma$ in (1), yielding:

$$\hat{\beta}^{\text{inv}} = \sigma^{-1} ||Y - X\beta||^2 + \lambda \Omega(\beta), \text{ where, } \sigma = \text{sdev}(\epsilon) \quad (4)$$

Estimating σ by $||Y - X\beta|| / \sqrt{n}$ and using the ℓ_1 penalty $\Omega(\beta) = ||\beta||_1$ leads to the $\sqrt{\text{Lasso}}$ estimator:

$$\hat{\beta}_\lambda^{\sqrt{\text{Lasso}}} = \underset{\beta \in \mathbb{R}^p}{\text{argmin}} \{ \sqrt{n} ||Y - X\beta|| + \lambda ||\beta||_1 \} \quad (5)$$

Clearly, the square-root Lasso estimator is scale-invariant and hence independent of the knowledge of σ , and still enjoys computational efficiency as the objective function is convex. The resulting estimator also enjoys near-oracle convergence rate, similar to Lasso, when $\text{supp}(\beta_0)$ has only s elements, $s < n$ [Belloni et al., 2011].

The square-root Lasso admits an alternative representation / algorithm, as another variant of Lasso called Scaled Lasso [Sun and Zhang, 2012], that establishes the connection between the original Lasso and the square-root Lasso. Following Giraud [2014], the square-root Lasso estimator in (5) and $\hat{\sigma} = ||Y - X\beta|| / \sqrt{n}$ can be written as solution to the convex system:

$$(\hat{\beta}, \hat{\sigma}) = \underset{\beta \in \mathbb{R}^p, \sigma \in \mathbb{R}^+}{\text{argmin}} \left\{ \frac{n\sigma}{2} + \frac{||Y - X\beta||^2}{2\sigma} + \lambda ||\beta||_1 \right\} \quad (6)$$

Hence, we have the following relationship between Lasso and the square-root Lasso estimators:

$$\hat{\beta}_\lambda^{\sqrt{\text{Lasso}}} = \hat{\beta}_{2\lambda\hat{\sigma}}^{\text{Lasso}}, \quad \text{where} \quad \hat{\sigma} = ||Y - X\beta|| / \sqrt{n}$$

This implies that the square-root Lasso (or, scaled Lasso) can be efficiently calculated by a scheme that alternately finds a Lasso estimate $\hat{\beta}$ and $\hat{\sigma}$, resulting in the scaled-Lasso algorithm

[[Sun and Zhang, 2012](#)].

Despite the attractive properties of these methods, there is a common caveat: the choice of tuning parameter λ . For Lasso, the tuning can be done either via a k -fold cross-validation or a complexity selection technique [[Giraud et al., 2012](#)]. However, these methods come with some concerns: while the k -fold CV works well empirically, it lacks theoretical support and the complexity selection is only guaranteed to work under Gaussianity of the data. The scale-invariant methods improve this situation slightly by making the tuning parameter free of σ , but it still requires tuning by adapting to the data.

Furthermore, it has been noted by some authors [[Chatterjee and Lahiri, 2011](#)] that the Lasso-based estimates do not yield meaningful standard errors for the parameter estimates, motivating full Bayesian treatment that produces reliable uncertainty quantification without extra effort. The Bayesian treatments of penalized regression depend on the useful duality of penalty and log-prior, and (Normal) scale mixture representation of the prior (e.g. Laplace as Normal-Gamma) that leads to efficient computation via EM/ECME or MCMC algorithms.

Our main contribution in this paper is a Bayesian interpretation of the square-root Lasso estimator based on the scale mixture representation of the Laplace density. Apart from quantifying uncertainty, this representation provides at least two alternative computational tools: via MCMC and via proximal algorithm [[Polson et al., 2015](#)]. We also offer new insights into the estimators behaviour by investigating the resulting posterior distribution and the shrinkage weights. The rest of the paper is organized as follows: §2 describes the Bayesian square-root Lasso, §3 provides some numerical examples and performance on a real data set, §4 provides some new theoretical results for the sparse regression problem and §5 concludes with future directions.

2 Bayesian $\sqrt{\text{Lasso}}$

2.1 Hierarchical Model

Here we derive the Bayesian hierarchical model corresponding to the $\sqrt{\text{Lasso}}$ in (5). Since the likelihood-prior decomposition of (5) yield a Laplace density for both the observation and the prior model, we use a Gaussian scale mixture representation of Laplace to write the Bayesian hierarchy.

The key step in the Bayesian hierarchy for $\sqrt{\text{Lasso}}$ follows from the well-known identity due to

Lévy [1940] given by:

$$\int_0^\infty \frac{a}{(2\pi)^{1/2} t^{3/2}} \exp\{-a^2/(2t)\} \exp\{-\lambda t\} dt = \exp\{-a(2\lambda)^{1/2}\}. \quad (7)$$

For deriving the full hierarchical model for $\sqrt{\text{Lasso}}$, we use $a = 1$, and $2\lambda = (\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^\top(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})$ to get

$$\exp\left[-\{(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^\top(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})\}^{1/2}\right] = \int_0^\infty \frac{1}{(2\pi)^{1/2} t^{3/2}} e^{-1/(2t)} e^{-\frac{1}{2}(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^\top(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})t} dt \quad (8)$$

To complete the hierarchy we use the normal scale mixture of Laplace prior on $\boldsymbol{\beta}$ [Andrews and Mallows, 1974] as follows:

$$\pi(\beta_i) \propto e^{-\tau|\beta_i|} = \int_0^\infty \frac{1}{\sqrt{2\pi}\lambda_i} e^{-\beta_i^2/(2\lambda_i^2)} \frac{\tau^2}{2} e^{-\lambda_i^2\tau^2/2} d\lambda_i^2 \quad i = 1, \dots, p.$$

The hyper-parameter τ serves the role of the tuning parameter in square-root Lasso. We can either estimate it via an empirical Bayes marginal maximum likelihood or use a Gamma hyperprior on τ to learn via full Bayes.

$$\pi(\tau^2) = \frac{\delta^r}{\Gamma(r)} (\tau^2)^{r-1} e^{-\delta\tau^2}, \quad \tau^2 > 0, \quad (r > 0, \delta > 0). \quad (9)$$

Under the Gamma hyper-prior, the joint distribution of y_i and all the hyperparameters in the model is :

$$f(\mathbf{y}, \boldsymbol{\beta}, t, \boldsymbol{\lambda}, \tau^2 \mid \mathbf{r}, \delta) \propto \frac{1}{t^{3/2}} \exp\{-1/(2t)\} \exp\left\{-\frac{1}{2}(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^\top(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})t\right\} \\ \prod_{i=1}^p (\lambda_i^2)^{-\frac{1}{2}} \exp\{-\beta_i^2/(2\lambda_i^2)\} \frac{\tau^2}{2} e^{-\lambda_i^2\tau^2/2} (\tau^2)^{r-1} e^{-\delta\tau^2} \quad (10)$$

The joint distribution in (16) provides the full hierarchical model for a Bayesian treatment. To maintain notational similarity, we first transform $t/2 = \sigma^{-2}$ and write the reparametrized joint distribution as:

$$f(\mathbf{y}, \boldsymbol{\beta}, \sigma^2, \boldsymbol{\lambda}, \tau^2 \mid \mathbf{r}, \delta) \propto \frac{1}{\sqrt{\sigma^2}} \exp\{-\sigma^2/(4)\} \exp\left\{-\frac{1}{2}(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})^\top(\mathbf{y} - \mathbf{X}\boldsymbol{\beta})/\sigma^2\right\} \\ \prod_{i=1}^p (\lambda_i^2)^{-\frac{1}{2}} \exp\{-\beta_i^2/(2\lambda_i^2)\} \frac{\tau^2}{2} e^{-\lambda_i^2\tau^2/2} (\tau^2)^{r-1} e^{-\delta\tau^2} \quad (11)$$

Hence the hierarchical representation of the full model is as follows:

$$\mathbf{y} \mid \boldsymbol{\beta}, \sigma^2 \sim \mathcal{N}(\mathbf{X}\boldsymbol{\beta}, \sigma^2 \mathbf{I}) \quad (12)$$

$$\boldsymbol{\beta} \sim \mathcal{N}(\mathbf{0}, D_\lambda), \quad D_\lambda = \text{Diag}(\lambda_1^2, \dots, \lambda_p^2) \quad (13)$$

$$\lambda_1^2, \dots, \lambda_p^2 \sim \prod_{j=1}^p \frac{\tau^2}{2} e^{-\lambda_j^2 \tau^2 / 2}, \quad \lambda_i^2 > 0, \quad (14)$$

$$\tau^2, \sigma^2 \sim (\tau^2)^{r-1} e^{-\delta \tau^2} \exp\{-\sigma^2 / (4)\}, \quad \tau^2, \sigma^2 > 0. \quad (15)$$

2.2 Gibbs Sampler

For simplicity, we show here the equations for the sparse Gaussian means model where \mathbf{X} is an identity matrix of suitable dimensions, rendering the joint distribution as:

$$f(\mathbf{y}, \boldsymbol{\beta}, t, \boldsymbol{\lambda}, \tau^2 \mid \mathbf{r}, \delta) \propto \frac{1}{t^{3/2}} \exp\{-1/(2t)\} \exp\left\{-\frac{1}{2} \sum_{i=1}^p (y_i - \beta_i)^2 t\right\} \\ \prod_{i=1}^p (\lambda_i^2)^{-\frac{1}{2}} \exp\{-\beta_i^2 / (2\lambda_i^2)\} \frac{\tau^2}{2} e^{-\lambda_i^2 \tau^2 / 2} (\tau^2)^{r-1} e^{-\delta \tau^2} \quad (16)$$

The full conditional distributions of β_i and τ are easy to derive: The full conditional of β_i is multivariate normal and τ is Gamma, exploiting the conjugacy. The parameters t and λ_i^2 follow inverse Gaussian distribution, where we assume the following parametric form of the inverse Gaussian density:

$$f(x \mid \lambda', \mu') = \sqrt{\frac{\lambda'}{2\pi}} x^{-3/2} \exp\left\{-\frac{\lambda'(x - \mu')^2}{2(\mu')^2 x^2}\right\}, \quad x > 0$$

The full conditional distributions needed for implementing a Gibbs sampler are:

$$\beta_i \mid y_i, \lambda_i, t \sim \mathcal{N}\left(y_i \frac{\lambda_i^2 t}{1 + t\lambda_i^2}, \frac{\lambda_i^2}{1 + t\lambda_i^2}\right), \quad i = 1, \dots, n, \quad (17)$$

$$t \mid \mathbf{y}, \boldsymbol{\beta} \sim \text{Inv-Gauss}(\mu' = 1/\sqrt{\sum_{i=1}^p (y_i - \beta_i)^2}, \lambda' = 1) \quad (18)$$

$$\lambda_i^2 \mid \beta_i, \tau \sim \text{Inv-Gauss}(\mu' = |\frac{\beta_i}{\tau}|, \lambda' = \beta_i^2) \quad (19)$$

$$\tau^2 \mid \boldsymbol{\lambda}, r, \delta \sim \text{Gamma}(n + r, \delta + \sum_{i=1}^p \lambda_i^2 / 2) \quad (20)$$

3 Simulation Study: Sparse Normal Means

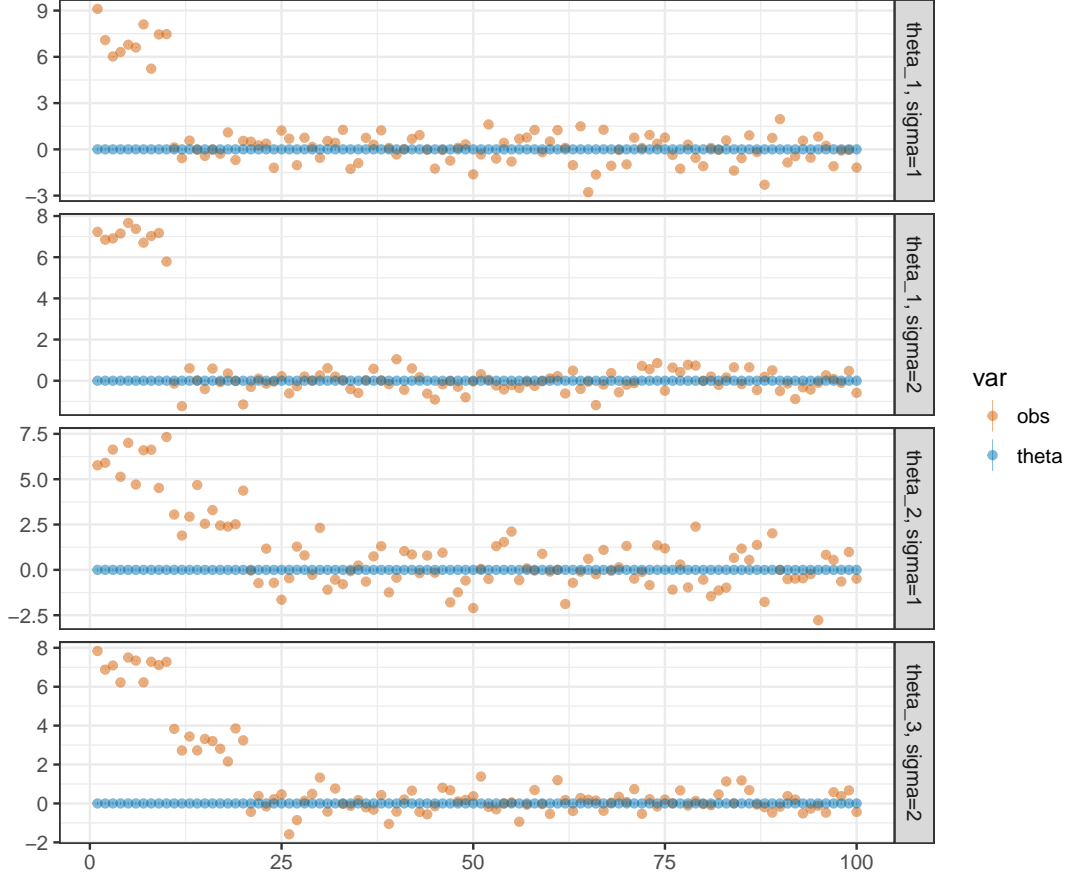


Figure 1: Comparison of posterior mean estimates for two different sparse normal means, $\beta_i \sim 0.8\delta_{\{7\}} + 0.1\delta_{\{3\}} + 0.1\delta_{\{0\}}$ and $\beta_i \sim 0.9\delta_{\{7\}} + 0.1\delta_{\{0\}}$ under the Bayesian $\sqrt{\text{Lasso}}$.

The Bayesian square-root Lasso method described above has sharpened ability to detect signals in a sparse regime. We demonstrate the sparse signal recovery of the Bayesian $\sqrt{\text{Lasso}}$ through a simulation study for estimating a sparse normal mean vector for two different choices of β :

1. $\beta = (\underbrace{7, \dots, 7}_{q_n=10}, \underbrace{0, \dots, 0}_{n-q_n=90})$ and
2. $\beta = (\underbrace{7, \dots, 7}_{q_n=10}, \underbrace{3, \dots, 3}_{r_n=10}, \underbrace{0, \dots, 0}_{n-q_n-r_n=80})$.

We generate observations from a Gaussian model $(y_i \mid \beta_i) \sim \mathcal{N}(\beta_i, \sigma^2)$ for $\sigma^2 = 1$ and $\sigma^2 = \frac{1}{2}$.

Figure 1 shows the posterior mean estimates for the four possible scenarios described above.

References

- D.F. Andrews and C.L. Mallows. Scale mixtures of normal distributions. *Journal of the Royal Statistical Society. Series B: Statistical Methodology*, 36(1):99–102, 1974. ISSN 00359246. doi: 10.2307/2984774.
- Alexandre Belloni, Victor Chernozhukov, and Lie Wang. Square-root lasso: Pivotal recovery of sparse signals via conic programming. *Biometrika*, 98(4):791–806, 2011.
- Peter J Bickel, Ya’acov Ritov, and Alexandre B Tsybakov. Simultaneous analysis of lasso and dantzig selector. *The Annals of Statistics*, pages 1705–1732, 2009.
- Peter Bühlmann and Sara van de Geer. *Statistics for High-Dimensional Data*. Springer-Verlag Berlin Heidelberg, 2011.
- A. Chatterjee and S. N. Lahiri. Bootstrapping lasso estimators. *Journal of the American Statistical Association*, 106(494):608–625, 2011. doi: 10.1198/jasa.2011.tm10159. URL <http://dx.doi.org/10.1198/jasa.2011.tm10159>.
- Bradley Efron, Trevor Hastie, Iain Johnstone, and Robert Tibshirani. Least angle regression. *The Annals of statistics*, 32(2):407–499, 2004. URL <http://projecteuclid.org/euclid.aos/1083178935>.
- Jerome Friedman, Trevor Hastie, Holger Höfling, Robert Tibshirani, and others. Pathwise coordinate optimization. *The Annals of Applied Statistics*, 1(2):302–332, 2007. URL <http://projecteuclid.org/euclid.aos/1196438020>.
- Christophe Giraud. *Introduction to high-dimensional statistics*, volume 138. CRC Press, 2014.
- Christophe Giraud, Sylvie Huet, Nicolas Verzelen, et al. High-dimensional regression with unknown variance. *Statistical Science*, 27(4):500–518, 2012.
- Paul Lévy. Sur certains processus stochastiques homogènes. *Compositio mathematica*, 7:283–339, 1940.
- Nicholas G Polson, James G Scott, and Brandon T Willard. Proximal algorithms in statistics and machine learning. *Statistical Science*, 30(4):559–581, 2015.
- Tingni Sun and Cun-Hui Zhang. Scaled sparse linear regression. *Biometrika*, 99(4):879–898, 2012.

R. Tibshirani. Regression Shrinkage and Selection via the Lasso. *Journal of the Royal Statistical Society. Series B*, 58:267–288, 1996.

Robert J Tibshirani. In praise of sparsity and convexity. *Past, Present, and Future of Statistical Science*, pages 497–505, 2014.