A tutorial on the LASSO and the "shooting algorithm"

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1 Abstract

The LASSO is an L_1 penalized regression technique introduced by Tibshirani [1996]. An efficient algorithm called the "shooting algorithm" was proposed by Fu [1998] for solving the LASSO problem in the multiparameter case. In this tutorial, we present a simple and self-contained derivation of the LASSO shooting algorithm.

2 Code distribution for LASSO shooting

MATLAB (www.mathworks.com) code for solving a LASSO problem using the "shooting algorithm" and estimating the regularization parameter can be downloaded from:

http://www.gautampendse.com/software/lasso/webpage/lasso_shooting.html

This software is freely made available under the creative commons attribution license:

http://creativecommons.org/licenses/by/3.0/

3 Notation

- Scalars will be denoted in a non-bold font possibly with subscripts (e.g. λ, β_i). We will use bold face lower case letters possibly with subscripts to denote vectors (e.g. y, x, β, z_1) and bold face upper case letters possibly with subscripts to denote matrices (e.g. X, B_1). The *i*th element of a vector x will be denoted by x_i in non-bold font.
- The transpose of a matrix X will be denoted by X^T and its inverse will be denoted by X^{-1} . We will denote the $p \times p$ identity matrix by I_p . A vector or matrix of all zeros will be denoted by a bold face zero $\mathbf{0}$ whose size should be clear from context.
- The q-norm of a $p \times 1$ vector $\boldsymbol{\beta}$ will be denoted by $||\boldsymbol{\beta}||_q = \left(\sum_{i=1}^p |\beta_i|^q\right)^{\frac{1}{q}}$ where $|\beta_i|$ denotes the absolute value of β_i .

4 Introduction

Given n feature vectors of length p arranged in the rows of a design matrix \mathbf{X} we would like to predict the $n \times 1$ observed response vector \mathbf{y} via a linear model. LASSO solves the following L_1

regularized optimization problem:

$$\min_{\boldsymbol{\beta}} h(\boldsymbol{\beta}) = \frac{1}{2} ||\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta}||_{2}^{2} + \lambda ||\boldsymbol{\beta}||_{1}, \text{ where } \lambda \ge 0$$
(4.1)

where
$$(4.2)$$

$$\boldsymbol{\beta}$$
 is a $p \times 1$ vector (4.3)

$$\mathbf{y}$$
 is a $n \times 1$ vector (4.4)

$$X$$
 is a $n \times p$ matrix (4.5)

We assume that n > p. The penalty term in 4.1 is a 1-norm penalty or simply the sum of the absolute values of the components of β . As we shall see, this penalty term encourages sparsity in the components of the solution vector β and thus automatically leads to feature/model selection. In addition, the penalty term regularizes the solution vector β and hence prevents overfitting.

5 Preliminaries

In this section, we give some background material that is necessary for a clear understanding of how LASSO works. We will cover some basic relationships between convexity, positive semidefiniteness, local and global minimizers.

Definition 5.1 (Convexity). A set \mathcal{D} is convex if for any $x_1, x_2 \in \mathcal{D}$ and all $\alpha \in (0,1)$, $x = \alpha x_1 + (1-\alpha)x_2 \in \mathcal{D}$. A function f(x) is convex if (1) its domain \mathcal{D} is convex and (2) $f(x) = f(\alpha x_1 + (1-\alpha)x_2) \leq \alpha f(x_1) + (1-\alpha)f(x_2)$.

Definition 5.2 (PSD). A $p \times p$ matrix \boldsymbol{H} is positive semidefinite (PSD) if for all $p \times 1$ vectors \boldsymbol{z} we have $\boldsymbol{z}^T \boldsymbol{H} \boldsymbol{z} \geq 0$.

Proposition 5.3 (PSD Hessian implies Convexity). Suppose \mathbf{x} is a $p \times 1$ vector and $f(\mathbf{x})$ is a scalar function of p variables with continuous second order derivatives defined on a convex domain \mathcal{D} . If the Hessian $\nabla^2 f(\mathbf{x})$ is positive semidefinite for all $x \in \mathcal{D}$ then f is convex.

Proof. By Taylor's theorem for all $x, x + h \in \mathcal{D}$ we can write:

$$f(\boldsymbol{x} + \boldsymbol{h}) = f(\boldsymbol{x}) + \nabla f(\boldsymbol{x})^T \boldsymbol{h} + \frac{1}{2} \boldsymbol{h}^T \nabla^2 f(\boldsymbol{x} + \theta \boldsymbol{h}) \boldsymbol{h}$$
 (5.1)

for some $\theta \in (0,1)$. By assumption, the Hessian $\nabla^2 f(\boldsymbol{x} + \theta \boldsymbol{h})$ is positive semidefinite and hence $\boldsymbol{h}^T \nabla^2 f(\boldsymbol{x} + \theta \boldsymbol{h}) \boldsymbol{h} \geq 0$. Hence for all $\boldsymbol{x}, \boldsymbol{x} + \boldsymbol{h} \in \mathcal{D}$ we can write:

$$f(\boldsymbol{x} + \boldsymbol{h}) \ge f(\boldsymbol{x}) + \nabla f(\boldsymbol{x})^T \boldsymbol{h}$$
(5.2)

Letting x + h = y we can also write the above equation as:

$$f(y) \ge f(x) + \nabla f(x)^T (y - x) \ \forall x, y \in \mathcal{D}$$
 (5.3)

Now let x_1 and x_2 be any two points in \mathcal{D} and let $\alpha \in (0,1)$ be a scalar. Then by the convexity of \mathcal{D} , $x = \alpha x_1 + (1 - \alpha)x_2 \in \mathcal{D}$.

By 5.3 we can write:

$$f(\mathbf{x}_1) \ge f(\mathbf{x}) + \nabla f(\mathbf{x})^T (\mathbf{x}_1 - \mathbf{x}) \tag{5.4}$$

and

$$f(\mathbf{x}_2) \ge f(\mathbf{x}) + \nabla f(\mathbf{x})^T (\mathbf{x}_2 - \mathbf{x})$$
(5.5)

Multiplying 5.4 by α and 5.5 by $(1 - \alpha)$ and adding we get:

$$\alpha f(\boldsymbol{x}_1) + (1 - \alpha) f(\boldsymbol{x}_2) \ge f(\boldsymbol{x}) + \nabla f(\boldsymbol{x})^T (\alpha \boldsymbol{x}_1 + (1 - \alpha) \boldsymbol{x}_2 - \boldsymbol{x})$$

$$= f(\boldsymbol{x})$$
(5.6)

Hence f(x) is convex.

Proposition 5.4. If f(x) and g(x) are convex functions defined on a convex domain \mathcal{D} then r(x) = f(x) + g(x) is also convex on \mathcal{D} .

Proof. Suppose $x_1, x_2 \in \mathcal{D}$ and let $x = \alpha x_1 + (1 - \alpha)x_2$ for some $\alpha \in (0, 1)$. Since \mathcal{D} is convex we have $x \in \mathcal{D}$. Now

$$r(\mathbf{x}) = r(\alpha \mathbf{x}_1 + (1 - \alpha)\mathbf{x}_2) \tag{5.7}$$

$$= f(\alpha \mathbf{x}_1 + (1 - \alpha)\mathbf{x}_2) + g(\alpha \mathbf{x}_1 + (1 - \alpha)\mathbf{x}_2)$$

$$(5.8)$$

$$\leq \alpha f(\boldsymbol{x}_1) + (1 - \alpha)f(\boldsymbol{x}_2) + \alpha g(\boldsymbol{x}_1) + (1 - \alpha)g(\boldsymbol{x}_2)$$
 by convexity of f and g (5.9)

$$= \alpha r(\boldsymbol{x}_1) + (1 - \alpha)r(\boldsymbol{x}_2) \tag{5.10}$$

Hence r(x) is convex.

Proposition 5.5 (LASSO objective is convex). The LASSO objective function $h(\beta)$ in equation 4.1 is convex.

Proof. We can write the LASSO objective as:

$$h(\beta) = f(\beta) + g(\beta) \tag{5.11}$$

where $f(\beta) = \frac{1}{2}||\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta}||_2^2$ and $g(\beta) = \lambda||\boldsymbol{\beta}||_1$. Note that the domain of both functions f and g is \mathbf{R}^p which is convex.

The Hessian of $f(\beta)$ is $\nabla^2 f(\beta) = \mathbf{X}^T \mathbf{X}$. For any $p \times 1$ vector \mathbf{z} : $\mathbf{z}^T \mathbf{X}^T \mathbf{X} \mathbf{z} = ||\mathbf{X} \mathbf{z}||_2^2 \ge 0$. Hence $\nabla^2 f(\beta)$ is positive semidefinite. Hence by proposition 5.3 $f(\beta)$ is convex.

For any β_1, β_2 and any $\alpha \in (0,1)$, let $\beta = \alpha \beta_1 + (1-\alpha)\beta_2$. Then

$$g(\boldsymbol{\beta}) = \lambda ||\alpha \boldsymbol{\beta}_1 + (1 - \alpha)\boldsymbol{\beta}_2||_1 \tag{5.12}$$

$$\leq \lambda ||\alpha \beta_1||_1 + \lambda ||(1 - \alpha)\beta_2||_1$$
 Triangle inequality (5.13)

$$= \lambda \alpha ||\boldsymbol{\beta}_1||_1 + \lambda (1 - \alpha) ||\boldsymbol{\beta}_2||_1 \tag{5.14}$$

$$= \alpha g(\boldsymbol{\beta}_1) + (1 - \alpha) g(\boldsymbol{\beta}_2) \tag{5.15}$$

Hence $g(\beta)$ is convex. Since $f(\beta)$ and $g(\beta)$ are both convex, by proposition 5.4 $h(\beta) = f(\beta) + g(\beta)$ is also convex.

Proposition 5.6. If f(x) is a convex function defined for $x \in \mathcal{D}$ with convex \mathcal{D} then any local minimizer of f on \mathcal{D} is a global minimizer of f on \mathcal{D} .

Proof. Suppose x^* is a local minimizer but not a global minimizer. Then there exists a global minimizer x_q^* such that:

$$f(\boldsymbol{x}_q^*) < f(\boldsymbol{x}^*) \tag{5.16}$$

In addition, since x^* is a local minimizer we must have:

$$f(\mathbf{y}) \ge f(\mathbf{x}^*) \text{ for all } \mathbf{y} \in \text{nbhd}(\mathbf{x}^*)$$
 (5.17)

Here $\mathrm{nbhd}(\boldsymbol{x}^*)$ is a local neighborhood of \boldsymbol{x}^* . By the convexity of f and \mathcal{D} , for any $\alpha \in (0,1)$ we can write:

$$f(\alpha \mathbf{x}^* + (1 - \alpha)\mathbf{x}_g^*) \le \alpha f(\mathbf{x}^*) + (1 - \alpha)f(\mathbf{x}_g^*)$$

$$(5.18)$$

$$< \alpha f(\boldsymbol{x}^*) + (1 - \alpha)f(\boldsymbol{x}^*)$$
 using 5.16 (5.19)

$$= f(\boldsymbol{x}^*) \tag{5.20}$$

For sufficiently small α such that $\mathbf{y} = \alpha \mathbf{x}^* + (1 - \alpha) \mathbf{x}_q^* \in \text{nbhd}(\mathbf{x}^*)$ we get:

$$f(y) < f(x^*) \text{ with } y \in \text{nbhd}(x^*)$$
 using 5.18 (5.21)

Comparing 5.17 and 5.21 we have a contradiction. Hence we must have $f(x_g^*) \ge f(x^*)$. However, since x_g^* is a global minimizer we must also have $f(x_g^*) \le f(x^*)$. Therefore we must have $f(x_g^*) = f(x^*)$. In other words, the local minimizer x^* is also a global minimizer as claimed.

Remark 5.7. Note that x^* is not necessarily equal to x_g^* in proposition 5.6. It is quite possible that $x^* \neq x_q^*$ but at the same time the convexity of f and \mathcal{D} will imply that $f(x_q^*) = f(x^*)$.

6 Derivation of the LASSO "shooting algorithm"

In this section, we present a simple derivation of the "shooting algorithm". First, we consider the case of single variable optimization, i.e., when p = 1. Next, we show how this simple case can be applied to the multi parameter situation via the "shooting algorithm".

6.1 Single variable case: p = 1

The optimization problem 4.1 is non-smooth because of the presence of the L_1 penalty term. We can convert this problem into a smooth one by introducing a new scalar variable t. The next proposition establishes the link between the two optimization problems.

Proposition 6.1. Suppose $\beta \in \mathbf{R}$ is a scalar and \mathbf{x} and \mathbf{y} are $n \times 1$ vectors. Consider the 1-D optimization problem

$$min_{\beta} h(\beta) = \frac{1}{2} ||\boldsymbol{y} - \boldsymbol{x}\beta||_2^2 + \lambda |\beta|, \text{ where } \lambda \ge 0$$
 (6.1)

Suppose β_1^* is the solution to 6.1. Consider another 1-D optimization problem:

$$min_{\beta} \bar{h}(\beta) = \frac{1}{2} ||\boldsymbol{y} - \boldsymbol{x}\beta||_{2}^{2} + \lambda t, \text{ where } \lambda \ge 0$$
 (6.2)

$$t - \beta \ge 0 \tag{6.3}$$

$$t + \beta \ge 0 \tag{6.4}$$

Suppose (β^*, t^*) is the solution to 6.2. Then $\beta^* = \beta_1^*$.

Proof. By proposition 5.5 the objective function in 6.1 is convex. Suppose (t_1, β_1) and (t_2, β_2) satisfy the constraints in 6.2. Then $t_1 - \beta_1 \ge 0$ and $t_1 + \beta_1 \ge 0$. Also $t_2 - \beta_2 \ge 0$ and $t_2 + \beta_2 \ge 0$. Now let $\alpha \in (0,1)$ and let $t = \alpha t_1 + (1-\alpha)t_2$ and $\beta = \alpha\beta_1 + (1-\alpha)\beta_2$. Then $t - \beta = \alpha(t_1 - \beta_1) + (1-\alpha)(t_2 - \beta_2) \ge 0$. Similarly, $t + \beta = \alpha(t_1 + \beta_1) + (1-\alpha)(t_2 + \beta_2) \ge 0$. Hence (t,β) also satisfy the constraints. This implies that the constraints define a convex set. The Hessian of the objective function in 6.2 is $H(\beta,t) = \begin{pmatrix} x_0^T x_0 \\ 0 \end{pmatrix}$. Clearly, this is positive semidefinite. Hence by proposition 5.3, the optimization problem in 6.2 is convex. Hence by proposition 5.6 any local minimizer of 6.1 or 6.2 is also a global minimizer.

Since (β^*, t^*) is the local (and hence global) solution of 6.2, for all (β, t) such that $t - \beta \ge 0$ and $t + \beta > 0$ we can write:

$$\frac{1}{2}||y - x\beta^*||_2^2 + \lambda t^* \le \frac{1}{2}||y - x\beta||_2^2 + \lambda t$$
(6.5)

In particular, $\beta = \beta_1^*$ and $t = |\beta_1^*|$ satisfy the constraints in 6.2 and hence we can write:

$$\frac{1}{2} ||\boldsymbol{y} - \boldsymbol{x}\beta^*||_2^2 + \lambda t^* \le \frac{1}{2} ||\boldsymbol{y} - \boldsymbol{x}\beta_1^*||_2^2 + \lambda |\beta_1^*|$$
(6.6)

Since β_1^* is a global minimizer of 6.1 we can write:

$$\frac{1}{2} ||\boldsymbol{y} - \boldsymbol{x}\beta_1^*||_2^2 + \lambda |\beta_1^*| \le \frac{1}{2} ||\boldsymbol{y} - \boldsymbol{x}\beta^*||_2^2 + \lambda |\beta^*|$$
(6.7)

Adding 6.6 and 6.7 and simplifying we get:

$$t^* \le |\beta^*| \tag{6.8}$$

But t^* satisfies $t^* \ge \beta^*$ and $t^* \ge -\beta^*$ i.e., $t^* \ge |\beta^*|$. From 6.8 we must therefore have:

$$t^* = |\beta^*| \tag{6.9}$$

Substituting 6.9 in 6.6 we get:

$$\frac{1}{2}||\boldsymbol{y} - \boldsymbol{x}\beta^*||_2^2 + \lambda|\beta^*| \le \frac{1}{2}||\boldsymbol{y} - \boldsymbol{x}\beta_1^*||_2^2 + \lambda|\beta_1^*|$$
(6.10)

From 6.10 and 6.7 we must have:

$$\frac{1}{2}||\boldsymbol{y} - \boldsymbol{x}\beta^*||_2^2 + \lambda|\beta^*| = \frac{1}{2}||\boldsymbol{y} - \boldsymbol{x}\beta_1^*||_2^2 + \lambda|\beta_1^*|$$
(6.11)

Expanding we get:

$$\frac{1}{2} \boldsymbol{y}^T \boldsymbol{y} + \frac{1}{2} (\beta^*)^2 \boldsymbol{x}^T \boldsymbol{x} - \boldsymbol{y}^T \boldsymbol{x} \beta^* + \lambda |\beta^*| = \frac{1}{2} \boldsymbol{y}^T \boldsymbol{y} + \frac{1}{2} (\beta_1^*)^2 \boldsymbol{x}^T \boldsymbol{x} - \boldsymbol{y}^T \boldsymbol{x} \beta_1^* + \lambda |\beta_1^*|$$
(6.12)

Case 1: $\lambda = 0$: In this case, $\frac{1}{2}||\boldsymbol{y} - \boldsymbol{x}\beta_1^*||_2^2 + \lambda|\beta_1^*| = \frac{1}{2}||\boldsymbol{y} - \boldsymbol{x}\beta_1^*||_2^2$ which is minimized for $\beta_1^* = \boldsymbol{y}^T \boldsymbol{x}/\boldsymbol{x}^T \boldsymbol{x}$. Similarly $\frac{1}{2}||\boldsymbol{y} - \boldsymbol{x}\beta^*||_2^2 + \lambda t^* = \frac{1}{2}||\boldsymbol{y} - \boldsymbol{x}\beta^*||_2^2$ which is minimized for $\beta^* = \boldsymbol{y}^T \boldsymbol{x}/\boldsymbol{x}^T \boldsymbol{x}$. Hence, in this case we have $\beta^* = \beta_1^* = \boldsymbol{y}^T \boldsymbol{x}/\boldsymbol{x}^T \boldsymbol{x}$.

Case 2: $\lambda \neq 0$ and $\mathbf{y}^T \mathbf{x} = 0$: In this case, $\frac{1}{2} ||\mathbf{y} - \mathbf{x} \beta_1^*||_2^2 + \lambda |\beta_1^*| = \frac{1}{2} \mathbf{y}^T \mathbf{y} + \frac{1}{2} (\beta_1^*)^2 \mathbf{x}^T \mathbf{x} + \lambda |\beta_1^*|$ which is minimized for $\beta_1^* = 0$. Similarly, $\frac{1}{2} ||\mathbf{y} - \mathbf{x} \beta^*||_2^2 + \lambda t^* = \frac{1}{2} ||\mathbf{y} - \mathbf{x} \beta^*||_2^2 + \lambda |\beta^*| = \frac{1}{2} \mathbf{y}^T \mathbf{y} + \frac{1}{2} (\beta^*)^2 \mathbf{x}^T \mathbf{x} + \lambda |\beta^*|$ which is minimized for $\beta^* = 0$. Hence, in this case we have $\beta^* = \beta_1^* = 0$.

Case 3: $\lambda \neq 0$ and $y^T x \neq 0$: Equation 6.12 holds for all values of λ , x and y. Equating the terms containing λ we must have:

$$|\beta^*| = |\beta_1^*| \tag{6.13}$$

Equation 6.13 already ensures that $\frac{1}{2}(\beta^*)^2 x^T x = \frac{1}{2}(\beta_1^*)^2 x^T x$. Equating the coefficient of $y^T x$ on both sides of 6.12 we get:

$$-\boldsymbol{y}^T \boldsymbol{x} \boldsymbol{\beta}^* = -\boldsymbol{y}^T \boldsymbol{x} \boldsymbol{\beta}_1^* \tag{6.14}$$

Since $\mathbf{y}^T \mathbf{x} \neq 0$, we must have $\beta^* = \beta_1^*$ which is consistent with 6.13.

Hence in all cases, we have $\beta^* = \beta_1^*$ as claimed.

Proposition 6.2. Consider another 1-D optimization problem:

$$min_{\beta} \ \bar{h}(\beta) = \frac{1}{2} ||\boldsymbol{y} - \boldsymbol{x}\beta||_{2}^{2} + \lambda t, \ where \ \lambda \ge 0$$
 (6.15)

$$t - \beta \ge 0 \tag{6.16}$$

$$t + \beta \ge 0 \tag{6.17}$$

Suppose $x \neq 0$ and suppose (β^*, t^*) is the solution to 6.15. Then β^* is given by:

$$\beta^* = \begin{cases} \frac{(\mathbf{y}^T \mathbf{x} - \lambda)}{\mathbf{x}^T \mathbf{x}} & \text{if } \mathbf{y}^T \mathbf{x} - \lambda > 0, \\ \frac{(\mathbf{y}^T \mathbf{x} + \lambda)}{\mathbf{x}^T \mathbf{x}} & \text{if } \mathbf{y}^T \mathbf{x} + \lambda < 0, \\ 0 & \text{if } -\lambda \le \mathbf{y}^T \mathbf{x} \le \lambda. \end{cases}$$
(6.18)

Proof. The Lagrangian for the optimization problem 6.15 is:

$$\mathcal{L}(\beta, t, \lambda_1, \lambda_2) = \frac{1}{2} ||\boldsymbol{y} - \boldsymbol{x}\beta||_2^2 + \lambda t - \lambda_1(t - \beta) - \lambda_2(t + \beta)$$
(6.19)

The Karush-Kuhn-Tucker (KKT) necessary conditions of optimality for (β^*, t^*) are:

$$\frac{\partial \mathcal{L}}{\partial \beta} = 0 \Longrightarrow \beta \, \boldsymbol{x}^T \boldsymbol{x} = \boldsymbol{y}^T \boldsymbol{x} + \lambda_2 - \lambda_1$$

$$\frac{\partial \mathcal{L}}{\partial t} = 0 \Longrightarrow \lambda_1 + \lambda_2 = \lambda$$

$$t - \beta \ge 0$$

$$t + \beta \ge 0$$
Inequality constraints
$$\lambda_1 \ge 0$$

$$\lambda_2 \ge 0$$
Positivity of λ_1, λ_2

$$\lambda_1(t - \beta) = 0$$

$$\lambda_2(t + \beta) = 0$$
Complementarity constraints
$$(6.20)$$

If $\mathbf{y}^T \mathbf{x} = 0$ then as shown in proposition 6.1 Case 1 and Case 2, $\beta^* = 0$. Thus we assume without loss of generality that $\mathbf{y}^T \mathbf{x} \neq 0$.

Case 1: $\mathbf{y}^T \mathbf{x} - \lambda > 0$: From 6.20 $\beta \mathbf{x}^T \mathbf{x} = \mathbf{y}^T \mathbf{x} + \lambda_2 - \lambda_1$ and $\lambda_1 + \lambda_2 = \lambda$. Thus $\beta \mathbf{x}^T \mathbf{x} = \mathbf{y}^T \mathbf{x} - \lambda + 2\lambda_2$. Since $\lambda_2 \geq 0$ (by 6.20) and $\mathbf{y}^T \mathbf{x} - \lambda > 0$ (by assumption in Case 1) we have that:

$$\beta \mathbf{x}^T \mathbf{x} = (\mathbf{y}^T \mathbf{x} - \lambda) + 2\lambda_2 > 0 \tag{6.21}$$

Since $x \neq 0$ we must have $\beta > 0$. Also, adding the inequality constraints in 6.20 we have $t \geq 0$. Hence in Case 1, we must have $(t + \beta) > 0$. Hence the complementarity constraints in 6.20 imply that $\lambda_2 = 0$. Hence from 6.21 we have:

$$\beta = \frac{(\mathbf{y}^T \mathbf{x} - \lambda)}{\mathbf{x}^T \mathbf{x}} \tag{6.22}$$

Case 2: $\mathbf{y}^T \mathbf{x} + \lambda < 0$: From 6.20 $\beta \mathbf{x}^T \mathbf{x} = \mathbf{y}^T \mathbf{x} + \lambda_2 - \lambda_1$ and $\lambda_1 + \lambda_2 = \lambda$. Thus $\beta \mathbf{x}^T \mathbf{x} = \mathbf{y}^T \mathbf{x} + \lambda - 2\lambda_1$. Since $\lambda_1 \geq 0$ (by 6.20) and $\mathbf{y}^T \mathbf{x} + \lambda < 0$ (by assumption in Case 2) we have that:

$$\beta \mathbf{x}^T \mathbf{x} = (\mathbf{y}^T \mathbf{x} + \lambda) - 2\lambda_1 < 0 \tag{6.23}$$

Since $x \neq 0$ we must have $\beta < 0$. Since $t \geq |\beta| \geq 0$, in Case 2, we must have $(t - \beta) > 0$. Hence the complementarity constraints in 6.20 imply that $\lambda_1 = 0$. Hence from 6.23 we have that:

$$\beta = \frac{(\mathbf{y}^T \mathbf{x} + \lambda)}{\mathbf{x}^T \mathbf{x}} \tag{6.24}$$

Case 3: $-\lambda \leq y^T x \leq \lambda$: If $\beta > 0$ then $(t+\beta) > 0$ which implies $\lambda_2 = 0$ (complementarity) and as in 6.22 $\beta = \frac{(y^T x - \lambda)}{x^T x}$. However $y^T x - \lambda \leq 0$ in Case 3 which means $\beta \leq 0$ which is a contradiction.

Similarly, if $\beta < 0$ then $(t - \beta) > 0$ which implies $\lambda_1 = 0$ (complementarity) and as in 6.24 $\beta = \frac{(\boldsymbol{y}^T \boldsymbol{x} + \lambda)}{\boldsymbol{x}^T \boldsymbol{x}}$. By assumption in Case 3 $\boldsymbol{y}^T \boldsymbol{x} + \lambda \geq 0$ which means $\beta \geq 0$ which is a contradiction.

The only way to avoid contradiction is to choose $\beta=0$ which leads to the following valid selection of lagrange multipliers:

$$\lambda_1 = \frac{\lambda + \boldsymbol{y}^T \boldsymbol{x}}{2} \ge 0 \tag{6.25}$$

$$\lambda_2 = \frac{\lambda - \boldsymbol{y}^T \boldsymbol{x}}{2} \ge 0 \tag{6.26}$$

It can be checked that $\beta = 0$, t = 0 and λ_1, λ_2 as given in 6.25 satisfy the all the KKT conditions of optimality in 6.20. Hence in all cases, β^* is given by 6.18 as claimed.

6.2 Multiple variable case: p > 1

In this section we describe the co-ordinate wise optimization approach of Fu [1998] which is also known as the "shooting algorithm" and show that it converges to the global minimum of the LASSO objective function.

The LASSO objective function is a sum of two convex functions one of which is non-differentiable. However, the non-differentiable part is separable in the individual co-ordinate wise components. As shown in Tseng [1988], for optimization problems with this structure, the co-ordinate wise optimization approach converges to a global minimum. This same property also holds in the case of blockwise co-ordinate optimization as shown in Tseng [2001]. As discussed in Friedman et al. [2007], a similar co-ordinate wise approach can also be applied to other methods related to LASSO such as the "elastic net".

Proposition 6.3. Consider the LASSO optimization problem:

$$min_{\boldsymbol{\beta}} h(\boldsymbol{\beta}) = \frac{1}{2} ||\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta}||_{2}^{2} + \lambda ||\boldsymbol{\beta}||_{1}, \text{ where } \lambda \ge 0$$
 (6.27)

Let $X = [x_1, x_2, \dots, x_p]$, $\beta = [\beta_1, \beta_2, \dots, \beta_p]^T$, $X^{(-i)} = [x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_p]$ and $\beta^{(-i)} = [\beta_1, \dots, \beta_{i-1}, \beta_{i+1}, \dots, \beta_p]^T$. Consider the following solution approach:

- Initialize $\beta = \beta_0$ (using for instance least squares, regularized least squares or randomly)
- For k = 0, 1, 2, ..., m repeat
 - Compute $f_k = h(\beta)$.
 - $For i = 1, 2, \dots, n$
 - 1. Using the current value of $\beta^{(-i)}$ solve the following 1-D optimization problem w.r.t. β_i

$$min_{\beta_i} h'(\beta_i) = \frac{1}{2} || \mathbf{y}_i - \mathbf{x}_i \beta_i ||_2^2 + \lambda |\beta_i| + \lambda || \boldsymbol{\beta}^{(-i)} ||_1$$
 (6.28)

where

$$\boldsymbol{y}_i = \boldsymbol{y} - \boldsymbol{X}^{(-i)} \boldsymbol{\beta}^{(-i)} \tag{6.29}$$

2. Suppose β_i^* is the solution to 6.28 then update the ith element of β to be equal to β_i^* i.e., set $\beta_i = \beta_i^*$

Then the sequence of iterates f_1, f_2, \ldots, f_m converge to the co-ordinate wise minimum of $h(\beta)$ in 6.27 as $m \to \infty$.

Proof. It is easy to see that:

$$h(\beta) = \frac{1}{2} ||y - X\beta||_2^2 + \lambda ||\beta||_1 = \frac{1}{2} ||y_i - x_i\beta_i||_2^2 + \lambda |\beta_i| + \lambda ||\beta^{(-i)}||_1$$
(6.30)

where y_i is defined in 6.29. If β_i^* solves the convex optimization problem 6.28 then we must have:

$$\frac{1}{2} || \boldsymbol{y}_i - \boldsymbol{x}_i \beta_i^* ||_2^2 + \lambda |\beta_i^*| + \lambda || \boldsymbol{\beta}^{(-i)} ||_1 \le \frac{1}{2} || \boldsymbol{y}_i - \boldsymbol{x}_i \beta_i ||_2^2 + \lambda |\beta_i| + \lambda || \boldsymbol{\beta}^{(-i)} ||_1 = h(\boldsymbol{\beta})$$
(6.31)

If β_{new} is the new vector obtained by updating the *i*th component of β to be equal to β_i^* then we can re-write 6.31 as:

$$h(\beta_{new}) \le h(\beta) \tag{6.32}$$

Hence we see that every iteration in the inner for loop (i = 1, 2, ..., p) decreases the objective function. This implies that:

$$f_{k+1} \le f_k \text{ for all } k \tag{6.33}$$

In addition f_k is bounded below by 0 i.e., $f_k \ge 0$ for all k. Suppose \hat{f} is the greatest lower bound on the sequence $\{f_k\}$. Then $\hat{f} \le f_k$ for all k. Choose any $\varepsilon > 0$. Then

$$f_k + \varepsilon > \hat{f} \tag{6.34}$$

Also $\hat{f} + \varepsilon$ is not the greatest lower bound. Hence there exists n_0 such that

$$f_{n_0} < \hat{f} + \varepsilon \tag{6.35}$$

Since $k > n_0$ implies $f_k \le f_{n_0}$ we conclude that:

$$f_k \le f_{n_0} < \hat{f} + \varepsilon \text{ if } k > n_0 \tag{6.36}$$

Hence for all $k > n_0$ we have:

$$\hat{f} - \varepsilon < f_k < \hat{f} + \varepsilon \tag{6.37}$$

In other words, the sequence $\{f_k\}$ converges to \hat{f} . If we cycle through all the co-ordinate directions until convergence then \hat{f} will be the co-ordinate wise minimum of $h(\beta)$.

Proposition 6.4. Suppose $\hat{\boldsymbol{\beta}}$ is the co-ordinate wise minimum of $h(\boldsymbol{\beta})$:

$$h(\hat{\beta} + \delta_i e_i) \ge h(\hat{\beta}) \text{ where } \delta_i \ne 0$$
 (6.38)

and e_i is a vector with a 1 at position i and zeros elsewhere. Then for any vector p in some open neighborhood of $\hat{\beta}$:

$$h(\hat{\boldsymbol{\beta}} + \boldsymbol{p}) \ge h(\hat{\boldsymbol{\beta}}) \tag{6.39}$$

i.e., $\hat{\beta}$ is a local minimizer of $h(\beta)$. Since $h(\beta)$ is convex this implies that $\hat{\beta}$ is also a global minimizer.

Proof. Recall that we can write the LASSO objective as:

$$h(\beta) = f(\beta) + g(\beta) \tag{6.40}$$

where

$$f(\boldsymbol{\beta}) = \frac{1}{2}||\boldsymbol{y} - \boldsymbol{X}\boldsymbol{\beta}||_2^2 \tag{6.41}$$

$$g(\boldsymbol{\beta}) = \lambda ||\boldsymbol{\beta}||_1 = \lambda \sum_{i=1}^p |\beta_i|$$
 (6.42)

Hence we can write:

$$h(\hat{\boldsymbol{\beta}} + \boldsymbol{p}) = f(\hat{\boldsymbol{\beta}} + \boldsymbol{p}) + g(\hat{\boldsymbol{\beta}} + \boldsymbol{p})$$
(6.43)

$$= f(\hat{\boldsymbol{\beta}}) + \boldsymbol{p}^T \nabla f(\hat{\boldsymbol{\beta}}) + \frac{1}{2} \boldsymbol{p}^T \boldsymbol{X}^T \boldsymbol{X} \boldsymbol{p} + \lambda \sum_{i=1}^p |\hat{\beta}_i + p_i|$$
(6.44)

$$= f(\hat{\boldsymbol{\beta}}) + \lambda \sum_{i=1}^{p} |\hat{\beta}_i| + \boldsymbol{p}^T \nabla f(\hat{\boldsymbol{\beta}}) + \frac{1}{2} \boldsymbol{p}^T \boldsymbol{X}^T \boldsymbol{X} \boldsymbol{p} + \lambda \sum_{i=1}^{p} |\hat{\beta}_i| + p_i| - \lambda \sum_{i=1}^{p} |\hat{\beta}_i|$$
(6.45)

$$= f(\hat{\boldsymbol{\beta}}) + g(\hat{\boldsymbol{\beta}}) + \boldsymbol{p}^T \nabla f(\hat{\boldsymbol{\beta}}) + \frac{1}{2} \boldsymbol{p}^T \boldsymbol{X}^T \boldsymbol{X} \boldsymbol{p} + \lambda \sum_{i=1}^p |\hat{\beta}_i + p_i| - \lambda \sum_{i=1}^p |\hat{\beta}_i|$$
(6.46)

$$=h(\hat{\boldsymbol{\beta}})+\boldsymbol{p}^{T}\nabla f(\hat{\boldsymbol{\beta}})+\frac{1}{2}\boldsymbol{p}^{T}\boldsymbol{X}^{T}\boldsymbol{X}\boldsymbol{p}+\lambda\sum_{i=1}^{p}|\hat{\beta}_{i}+p_{i}|-\lambda\sum_{i=1}^{p}|\hat{\beta}_{i}|$$
(6.47)

(6.48)

Let $p = \delta_i e_i$ in 6.43 with $\delta_i \neq 0$ then we can write:

$$h(\hat{\boldsymbol{\beta}} + \delta_i \boldsymbol{e}_i) = h(\hat{\boldsymbol{\beta}}) + \delta_i \boldsymbol{e}_i^T \nabla f(\hat{\boldsymbol{\beta}}) + \frac{1}{2} \delta_i^2 \boldsymbol{e}_i^T \boldsymbol{X}^T \boldsymbol{X} \boldsymbol{e}_i + \lambda |\hat{\beta}_i + \delta_i| - \lambda |\hat{\beta}_i|$$
(6.49)

By assumption $h(\hat{\beta} + \delta_i e_i) \ge h(\hat{\beta})$ and so we must have:

$$\delta_{i} \boldsymbol{e}_{i}^{T} \nabla f(\hat{\boldsymbol{\beta}}) + \frac{1}{2} \delta_{i}^{2} \boldsymbol{e}_{i}^{T} \boldsymbol{X}^{T} \boldsymbol{X} \boldsymbol{e}_{i} + \lambda |\hat{\beta}_{i} + \delta_{i}| - \lambda |\hat{\beta}_{i}| \ge 0$$

$$(6.50)$$

The above relationship holds for all δ_i not matter how small. By choosing $|\delta_i|$ sufficiently small, we can make the term $\frac{1}{2}\delta_i^2 \boldsymbol{e}_i^T \boldsymbol{X}^T \boldsymbol{X} \boldsymbol{e}_i$ arbitrarily close to 0. Hence there exists $\theta_i > 0$ such that for all $\delta_i \in (-\theta_i, \theta_i)$ the following holds:

$$\delta_i \mathbf{e}_i^T \nabla f(\hat{\boldsymbol{\beta}}) + \lambda |\hat{\beta}_i + \delta_i| - \lambda |\hat{\beta}_i| \ge 0$$
(6.51)

Now let

$$\mathbf{p} = \sum_{i=1}^{p} \delta_i \mathbf{e}_i \tag{6.52}$$

then from 6.43 we get:

$$h(\hat{\boldsymbol{\beta}} + \boldsymbol{p}) = h(\hat{\boldsymbol{\beta}}) + \sum_{i=1}^{p} \delta_{i} \boldsymbol{e}_{i}^{T} \nabla f(\hat{\boldsymbol{\beta}}) + \frac{1}{2} \boldsymbol{p}^{T} \boldsymbol{X}^{T} \boldsymbol{X} \boldsymbol{p} + \lambda \sum_{i=1}^{p} |\hat{\beta}_{i} + \delta_{i}| - \lambda \sum_{i=1}^{p} |\hat{\beta}_{i}|$$
(6.53)

Note that 6.51 implies:

$$\sum_{i=1}^{p} \delta_i e_i^T \nabla f(\hat{\boldsymbol{\beta}}) + \lambda \sum_{i=1}^{p} |\hat{\beta}_i + \delta_i| - \lambda \sum_{i=1}^{p} |\hat{\beta}_i| \ge 0$$

$$(6.54)$$

Therefore from 6.53 and 6.54 we must have:

$$h(\hat{\boldsymbol{\beta}} + \boldsymbol{p}) = h(\hat{\boldsymbol{\beta}}) + \sum_{i=1}^{p} \delta_{i} \boldsymbol{e}_{i}^{T} \nabla f(\hat{\boldsymbol{\beta}}) + \frac{1}{2} \boldsymbol{p}^{T} \boldsymbol{X}^{T} \boldsymbol{X} \boldsymbol{p} + \lambda \sum_{i=1}^{p} |\hat{\beta}_{i} + \delta_{i}| - \lambda \sum_{i=1}^{p} |\hat{\beta}_{i}|$$
(6.55)

$$\geq h(\hat{\boldsymbol{\beta}}) + \frac{1}{2} \boldsymbol{p}^T \boldsymbol{X}^T \boldsymbol{X} \boldsymbol{p} \tag{6.56}$$

$$\geq h(\hat{\boldsymbol{\beta}})$$
 by the positive semi-definiteness of $\boldsymbol{X}^T \boldsymbol{X}$ (6.57)

In other words, we have found an open neighborhood with $\delta_i \in (-\theta_i, \theta_i)$, $\theta_i > 0$ such that for all \boldsymbol{p} of the form 6.52, $h(\hat{\boldsymbol{\beta}} + \boldsymbol{p}) \geq h(\hat{\boldsymbol{\beta}})$. This implies that the co-ordinate wise minimizer $\hat{\boldsymbol{\beta}}$ is actually a local minimizer (and hence by convexity a global minimizer) of $h(\boldsymbol{\beta})$.

7 How to choose λ ?

The L_1 regularization parameter for LASSO can be chosen using cross validation. In brief, given data $(\boldsymbol{X}, \boldsymbol{y})$, we partition the rows of \boldsymbol{X} and \boldsymbol{y} into K parts giving us K data/response pairs: $(\boldsymbol{X}_1, \boldsymbol{y}_1), (\boldsymbol{X}_2, \boldsymbol{y}_2), \dots, (\boldsymbol{X}_K, \boldsymbol{y}_K)$. Let $(\boldsymbol{X}^{(-i)}, \boldsymbol{y}^{(-i)})$ be the data/response pair obtained by deleting the ith part $(\boldsymbol{X}_i, \boldsymbol{y}_i)$ from $(\boldsymbol{X}, \boldsymbol{y})$. Let $\beta_{lasso}^{(-i)}$ be the LASSO solution obtained using $(\boldsymbol{X}^{(-i)}, \boldsymbol{y}^{(-i)})$. Let n_i be the number of data points in the ith data/response pair $(\boldsymbol{X}_i, \boldsymbol{y}_i)$. For a given value of λ define the average cross validated mean squared error as:

$$\overline{CV}_{MSE}(\lambda) = \frac{1}{K} \sum_{i=1}^{K} \frac{1}{n_i} \left\| \left(\boldsymbol{y}_i - \boldsymbol{X}_i \, \boldsymbol{\beta}_{lasso}^{(-i)} \right) \right\|_2^2$$
(7.1)

Given a range of palusible values for λ we choose the optimal λ as the one that minimizes the average cross validated mean squared error:

$$\lambda^* = \arg\min_{\lambda} \overline{CV}_{MSE}(\lambda) \tag{7.2}$$

Figure 1 shows the process of choosing λ for an example data set using 10-fold cross-validation. Figure 2 shows the optimal LASSO fit using λ^* from Figure 1 as well as the estimated LASSO coefficients.

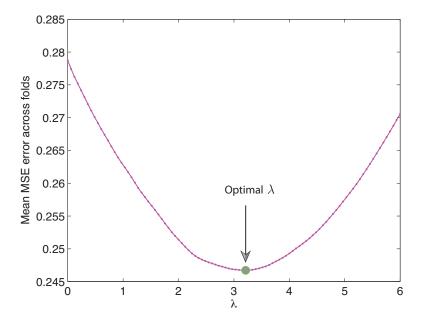


Figure 1: Average mean squared error across cross-validation folds (10-fold cross-validation) versus the regularization parameter λ for an example data set. Arrow shows the location of λ^* .

8 Conclusions

This goal of this tutorial was to provide a simple yet self-contained introduction to the LASSO [Tibshirani, 1996] technique for L_1 regularized linear regression. We discussed an efficient algorithm for optimizing the LASSO objective function - the "shooting algorithm" of Fu [1998]. From a practical point of view, we suggest a cross-validation based approach for choosing the regularization parameter λ . We encourage the reader to learn more about LASSO by visiting Rob Tibshirani's LASSO page: http://www-stat.stanford.edu/~tibs/lasso.html.

MATLAB code for estimating a LASSO model along with example data can be downloaded from: http://www.gautampendse.com/software/lasso/webpage/lasso_shooting.html.

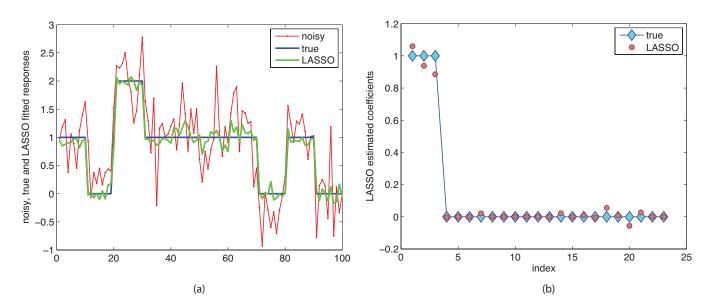


Figure 2: (a) Overlay of noisy data, true data and the LASSO fit obtained using λ^* from Figure 1 (b) The true coefficients versus the LASSO estimated coefficients using λ^* from Figure 1.

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