# Shrinkage Methods to Sparse Linear Regression

Main ref.:T. Hastie, R. Tibshirani, and J. Friedman,

The Elements of Statistical Learning 2nd Edition, Springer 2008 [1]

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#### **Abstract**

In this report, we introduce linear regression approaches using shrinkage methods. The shrinkage method have got attention to solve the problem of linear systems y = Ax because the method enables us to obtain the solution with lower variance than the conventional least square estimator having the minimum variance unbiasedness. First we will introduce basic concept of two shrinkage methods in the linear regression, *ridge and lasso*. Then, we move our focus to problems of the Lasso variants such as *Fused lasso* and *Elastic-net*. For the discussion in this report, we have partially referred to the chapter 3 of the book [1].

## I. INTRODUCTION

A linear regression problem starts from an assumption that the corresponding regression function  $\underline{Y} = f(\underline{X})$  is linear where  $\underline{Y} \in \mathbb{R}^M$  is a measurement vector generated by the function  $f(\cdot)$  given a vector  $\underline{X} \in \mathbb{R}^N$ . This assumption allows us to describe the function  $f(\cdot)$  using a linear projection, given by

$$\underline{Y} = \mathbf{A}\underline{X} \in \mathbb{R}^M,\tag{1}$$

where a measurement matrix  $\mathbf{A} \in \mathbb{R}^{M \times N}$  specifies the linear relation between  $\underline{Y}$  and  $\underline{X}$ . In such a regression problem, a typical aim is to estimate the unknown vector  $\underline{X}$  from a set of known inputs or training data  $(Y_1, \underline{a}_{\text{1st-row}})$  ...  $(Y_M, \underline{a}_{\text{Mst-row}})$  where  $\underline{a}_{\text{ith-row}} = [a_{j1}, a_{j2}, ..., a_{jN}]$  denotes the j-th row vector

of the matrix **A**. In addition, as before, we confine our focus to the linear regression problems which is underdetermined (M < N) such that there exists infinitely many solutions for  $\underline{X}$ .

The most standard approach to the linear regression problems is *least square estimation* (LSE). LSE obtains its estimate by solving the following optimization problem, given by

$$(P_{LSE}) : \underline{\widehat{X}}_{LSE} = \arg\min_{\underline{X}} \|\underline{Y} - \mathbf{A}\underline{X}\|_{2}^{2}$$

$$= \arg\min_{\underline{X}} \sum_{j=1}^{M} \left( Y_{j} - \sum_{i=1}^{N} a_{ji} X_{i} \right)^{2}.$$

$$(2)$$

It is well known that the LSE solver obtains an estimate  $\widehat{\underline{X}}_{LSE}$  by projecting the measurement vector  $\underline{Y}$  to a subspace of  $\mathbb{R}^M$  spanned by the column vectors of the matrix  $\mathbf{A}$ . Namely, the minimization task in (2) chooses  $\widehat{\underline{X}}_{LSE}$  which makes the vector difference  $\underline{Y} - \mathbf{A}\widehat{\underline{X}}_{LSE}$  to be orthogonal to the subspace. Such a LSE solution can be represented as a linear function of the measurement vector, *i.e.*,

$$\underline{\widehat{X}}_{LSE} = (\mathbf{A}^T \mathbf{A})^{-1} \mathbf{A}^T \underline{Y}.$$
 (3)

The popularity of LSE is originated from the Gauss-Markov theorem, one of the famous results in statistics. The Gauss-Markov theorem states that the LSE solver provides the smallest variance among all linear unbiased estimators. Let  $\underline{\widetilde{X}}$  denote an unbiased linear estimate, *i.e.*,  $E\left[\underline{\widetilde{X}}\right] = \underline{X}$ . The mean squared error (MSE) of  $\underline{\widetilde{X}}$  is calculated as

$$MSE\left(\underline{\widetilde{X}}\right) := E\left[\left(\underline{\widehat{X}} - \underline{X}\right)^{2}\right] = Var\left(\underline{\widetilde{X}}\right) + \left(E\left[\underline{\widehat{X}}\right] - \underline{X}\right)^{2}$$
$$= Var\left(\underline{\widetilde{X}}\right). \tag{4}$$

Then, the Gauss-Markov theorem shows that

$$\operatorname{Var}\left(\underline{\widehat{X}}_{LSE}\right) \le \operatorname{Var}\left(\underline{\widetilde{X}}\right) \tag{5}$$

for any other unbiased linear estimate  $\underline{\widetilde{X}}$  (We omit the proof here. please refer to [1]).

However, there may exist a biased estimator which can offer smaller MSE then the LSE solver. Such an estimator would provide a significant reduction in MSE at the expense of losing the unbiasedness [1],[3]. This is one motivation to use the shrinkage method to linear regression problem. The shrinkage methods is a biased estimation approach to impose a penalty to the optimization setting of (2). If the imposed penalty can properly catch the characteristic of the target unknown  $\underline{X}$ , the shrinkage methods greatly improve the estimation accuracy. In this report, we first introduce two types of the most well-known shrinkage methods, ridge and lasso, by partially referring to [1],[3]. Then, we extend our discussion to shrinkage methods which estimates the vector X having piecewise smooth or correlated property.

## II. SHRINKAGE WITH RIDGE PENALTY

In ridge regression, the elements of  $\underline{X}$  are shrunk by imposing a penalty on the energy of  $\underline{X}$  [2]. Therefore, the ridge penalty takes a quadratic form of  $\underline{X}$ , leading to the following optimization setup

$$(P_{\text{Ridge}}) : \underline{\widehat{X}}_{\text{Ridge}} = \arg\min_{\underline{X}} \|\underline{Y} - \mathbf{A}\underline{X}\|_{2}^{2} + \lambda \|\underline{X}\|_{2}^{2}$$

$$= \sum_{j=1}^{M} \left( y_{j} - \sum_{i=1}^{N} a_{ji} X_{i} \right)^{2} + \lambda \sum_{i=1}^{N} X_{i}^{2},$$

$$(6)$$

where  $\lambda \geq 0$  denote a parameter to control the amount of ridge shrinkage. Note that by applying the quadratic penalty  $\|\underline{X}\|_2^2 = \underline{X}^T \underline{X}$ , the ridge estimation can be represented as a closed form function of  $\underline{Y}$  if  $M \geq N$ , given by

$$\widehat{\underline{X}}_{\text{Ridge}} = (\mathbf{A}^T \mathbf{A} + \lambda \mathbf{I}_N)^{-1} \mathbf{A}^T \underline{Y}.$$
 (7)

This imposition of the ridge penalty adds a positive constant to the diagonal  $\mathbf{A}^T \mathbf{A}$  in (7) before inversion. It is noteworthy that this addition makes the regression problem nonsingular even when  $\mathbf{A}^T \mathbf{A}$  does not have full rank. Namely, the ridge solution is necessarily unique regardless of the condition of the matrix  $\mathbf{A}$ . This is a strong motivation to use ridge regression.

Ridge regression shrinks the coordinate of  $\underline{\widehat{X}}_{Ridge}$  according to the singular value of the matrix **A**. The singular value decomposition (SVD) of **A** has the form

$$\mathbf{A} = \mathbf{U}\mathbf{D}\mathbf{V}^T,\tag{8}$$

where  $\mathbf{U} \in \mathbb{R}^{M \times N}$  and  $\mathbf{V} \in \mathbb{R}^{N \times N}$  are orthogonal matrices, and  $\mathbf{D} \in \mathbb{R}^{N \times N}$  is a diagonal matrix with singular values  $d_1 \geq d_2 \geq ... \geq d_N \geq 0$  of  $\mathbf{A}$ . By applying SVD to the ridge solution, we can efficiently compute a ridge estimate  $\widehat{\underline{X}}_{\text{Ridge}}$  associated with the orthonormal basis  $\mathbf{U}$  and  $\mathbf{V}$ , as LSE does using the QR decomposition

$$\frac{\widehat{X}_{\text{Ridge}}}{\widehat{Y}_{\text{Ridge}}} = (\mathbf{A}^T \mathbf{A} + \lambda \mathbf{I}_N)^{-1} \mathbf{A}^T \underline{Y}$$

$$= \mathbf{V} (\mathbf{D}^2 + \lambda \mathbf{I}_N)^{-1} \mathbf{D} \mathbf{U}^T \underline{Y}$$

$$= \sum_{i=1}^{N} \underline{v}_i \frac{d_i}{d_i^2 + \lambda} \underline{u}_i^T \underline{Y}, \tag{9}$$

where the  $\underline{u}_i \in \mathbb{R}^M$  and  $\underline{v}_i \in \mathbb{R}^N$  are the column vectors of  $\mathbf{U}$  and  $\mathbf{V}$  respectively. In (9), ridge regression shrinks the elements of  $\underline{\widehat{X}}_{\text{Ridge}}$  by the factors  $d_i/(d_i^2 + \lambda)$ . This means that a greater amount of shrinkage is applied to the elements of  $\underline{\widehat{X}}_{\text{Ridge}}$  associated with  $\underline{v}_i$  having smaller singular values  $d_i$ . Namely, ridge

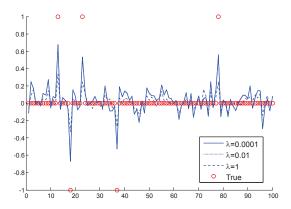


Fig. 1. Sparse estimation via ridge estimator with different  $\lambda$  where N = 100, M = 70, K = 5

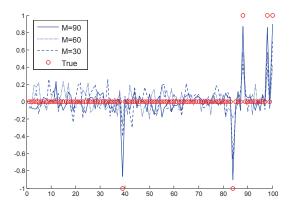


Fig. 2. Sparse estimation via ridge estimator with different M where  $N=100, K=5, \lambda=0.001$ 

regression shrinks together the correlated elements with  $\underline{v}_i$  if the direction of  $\underline{v}_i$  has small energy in the column space of  $\mathbf{A}$ .

The ridge penalty can be used to estimate sparse vectors  $\underline{X} \in \mathbb{R}^N$  in undetermined systems  $\underline{Y} = \mathbf{A}\underline{X} \in \mathbb{R}^M$ . In order to apply the expression of (7), we need an augmented matrix  $\mathbf{A}' \in \mathbb{R}^{N \times N}$  which additionally includes N-M zero rows from  $\mathbf{A} \in \mathbb{R}^{M \times N}$ . Let us consider sparse vectors  $\underline{X}$  which contains K nonzero signed elements having unit magnitude. The ridge penalty shrinks the elements of  $\underline{X}$  with respect to non-principal basis of  $\mathbf{A}'$ . Hence, the ridge regression enables the K largest elements, which are most related to the principal basis of  $\mathbf{A}'$ , to have exceptionally large magnitude.

We examine the ridge regression on the parameter N=100, K=5 with standard Gaussian matrix  $a_{ji} \in \mathbf{A} \sim \mathcal{N}(0, 1/M)$ . Fig.1 shows that the ridge estimation can finds the K largest elements of  $\underline{X}$  with appropriately chosen  $\lambda$ . Another example is shown in Fig.2 where we show the behavior of ridge regression according to the number of M. We note in Fig.2 that the magnitude of the K largest elements

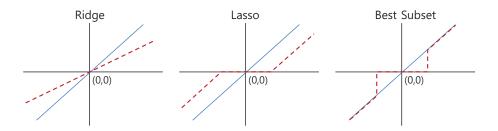


Fig. 3. Shrinkage characteristic of Ridge, Lasso and Best subset selection where the orthonomal matrix  $\mathbf{A}$  is assumed. In addition, the blue solid line in the figure is the  $45^{\circ}$  line to show the LSE solution as a reference (The figure is borrowed from Table 3.4 of [1]).

of  $\widehat{\underline{X}}$  becomes smaller as M decreases. This means that for clear distinction of the K largest elements, the ridge method requires M close to N. In addition, we know from Fig.1 and Fig.2 that the ridge solver cannot exactly fit the nonzero elements of  $\underline{X}$ .

# III. SHRINKAGE WITH LASSO PENALTY

The main characteristic of lasso is that the elements of  $\underline{X}$  are shrunk by imposing a  $L_1$ -norm penalty of  $\underline{X}$  [3]. Namely, the penalty in the lasso setup takes an absolute sum of  $\underline{X}$ , *i.e.*,  $\|\underline{X}\|_1 = \sum_{i=1}^N |X_i|$ . Following that, its optimization setup is represented as

$$(P_{\text{Lasso}}) : \underline{\widehat{X}}_{\text{Lasso}} = \arg\min_{\underline{X}} \|\underline{Y} - \mathbf{A}\underline{X}\|_{2}^{2} + \lambda \|\underline{X}\|_{1}$$

$$= \sum_{i=1}^{M} \left(y_{j} - \sum_{i=1}^{N} a_{ji}X_{i}\right)^{2} + \lambda \sum_{i=1}^{N} |X_{i}|,$$

$$(10)$$

where  $\lambda$  is a parameter to control the amount of lasso shrinkage. The larger  $\lambda$  leads to the stronger shrinkage against the elements of  $\underline{X}$ . When  $\lambda = 0$  the solution is equivalent to the LSE solution. This  $L_1$  penalty generates the solutions of (19) nonlinear with respect to the measurement vector  $\underline{Y}$ ; therefore, there is no closed form solver as in ridge regression. The lasso solver can be implemented via a quadratic programming. In addition, the *LARs* algorithm is well known as a computationally efficient algorithm for the lasso solution [4].

To see the detail of the lasso behavior, we investigate the Karush-Kuhn-Tucker (KKT) condition with

the Lagrangian  $\mathcal{L}(\underline{X}, \lambda)$  of the setup in (19).

- 1) Stationarity:  $\nabla_X \mathcal{L}(\underline{X}, \lambda) = \mathbf{G}\underline{X} \mathbf{A}^T\underline{Y} + \lambda\underline{B} = 0$ ,
- 2) Dual feasibility:  $\lambda \geq 0$ ,
- 3) Prime feasibility:  $\nabla_{\lambda} \mathcal{L}(\underline{X}, \lambda) = ||\underline{X}||_1 \leq 0$ ,
- 4) Complementary slackness for strong duality:  $\lambda \|\underline{X}\|_1 = 0$ , (11)

where we define a Gram matrix  $G := A^T A$  and

$$\underline{B} := \nabla_{\underline{X}} \|\underline{X}\|_1 = \left[ \frac{\partial \sum |X_i|}{\partial X_1}, \frac{\partial \sum |X_i|}{\partial X_2}, ..., \frac{\partial \sum |X_i|}{\partial X_N} \right]. \tag{12}$$

Since  $\sum |X_i|$  is not differentiable, we apply the concept of sub-differential to  $\frac{\partial \sum |X_i|}{\partial X_1}$ . Then, each element of  $\underline{B}$  is given by

$$B_{i} = \frac{\partial \sum |X_{i}|}{\partial X_{1}} := \begin{cases} \operatorname{sign}(X_{i}) & \text{if } |X_{i}| \geq \lambda \\ B_{i} \in [-1, 1] & \text{if } |X_{i}| < \lambda \end{cases}$$
 (13)

We note the stationarity condition in (11), which can be rewritten as

$$\mathbf{A}^T Y - \lambda B = \mathbf{G} X. \tag{14}$$

Insight about the lasso shrinkage can be obtained by assuming that the matrix A is orthonomal. By applying the orthonomal assumption to (14), we have

$$\widehat{\underline{X}}_{\text{Lasso}} = \mathbf{A}^T \underline{Y} - \lambda \underline{B}. \tag{15}$$

Then, the expression in (15) can be represented by a soft thresholding function with the parameter  $\lambda$  [5], *i.e.*,

$$\widehat{\underline{X}}_{\text{Lasso}} = \eta \left( \mathbf{A}^T \underline{Y}; \lambda \right), \tag{16}$$

where the thresholding function  $\eta(\tau; \lambda)$  is elementwisely defined as

$$\eta(\tau_i; \lambda) = \begin{cases}
\tau_i - \lambda & \text{if } \tau \ge \lambda_i, \\
\tau_i + \lambda & \text{if } \tau \le -\lambda_i, \\
0 & \text{otherwise.} 
\end{cases}$$
(17)

We know from (17) that lasso shrinks the elements of  $\underline{X}$  according to their magnitude. For the comparison purpose, we also consider ridge estimate with the orthonormal matrix  $\mathbf{A}$ , given by

$$\widehat{\underline{X}}_{\text{Ridge}} = \frac{1}{1+\lambda} \mathbf{A}^T \underline{Y}.$$
 (18)

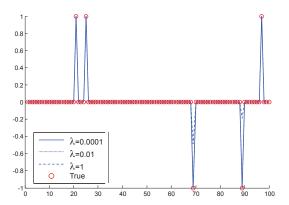


Fig. 4. Sparse estimation via lasso estimator with different  $\lambda$  where N=100, M=70, K=5

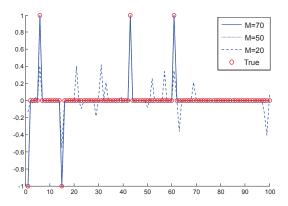


Fig. 5. Sparse estimation via lasso estimator with different M where  $N=100, K=5, \lambda=0.001$ 

Differently from the lasso case, the ridge estimate is obtained with a proportional shrinkage  $\frac{1}{1+\lambda}$  (radically the proportional shrinkage of ridge is determined by singular values of  $\mathbf{A}$ ). We borrow Fig.3 from the reference book (the figure in Table 3.4 of [1]) to depict the shrinkage characteristic of ridge and lasso, compared to the best subset selection which is an optimal estimator to find the  $K(\leq M)$  largest elements of  $\underline{X} \in \mathbb{R}^N$ . Fig.3 explicitly shows the difference among those three estimators.

We examine the lasso solver to estimate the signed K-sparse vectors  $\underline{X} \in \mathbb{R}^N$  from the undetermined system  $\underline{Y} = \mathbf{A}\underline{X} \in \mathbb{R}^M$ , as in the ridge regression. Fig.4 shows that the lasso solver perfectly finds the K largest elements with appropriate  $\lambda$ . We note in Fig.4 that the lasso estimate of the case  $\lambda = 1$  does not fit to the true of  $\underline{X}$  because in this case, the lasso penalty shrinks the elements too much. Fig.5 shows the lasso recovery of  $\underline{X}$  for a variety of the number of measurements M. In the figure, we see that the lasso solver finds an accurate solution when M = 50, 70, but fails in the estimation when M = 20.

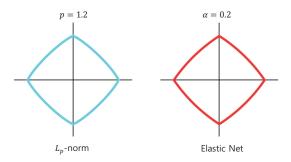


Fig. 6. Contours of the  $L_p$  penalty for p = 1.2 (left plot) and the elastic-net penalty ( $\alpha = 0.2$ ) (right plot) (The figure is borrowed from Figure 3.13 of [1].)

#### IV. VARIANTS OF LASSO

# A. Elastic-Net for Correlated Signal

We can generalize the ridge and the lasso penalty by using the concept of  $L_p$ -norm, i.e.,

$$(P_{L_p}): \underline{\widehat{X}}_{L_p} = \arg\min_{\underline{X}} \sum_{j=1}^{M} \left( y_j - \sum_{i=1}^{N} a_{ji} X_i \right)^2 + \lambda \sum_{i=1}^{N} |X_i|^p,$$
(19)

for  $p \ge 0$ , where the case p = 0 corresponds to the best subset selection which is non-convex; p = 2 corresponds to ridge regression which is convex; p = 1 is the lasso case which has the smallest p such that the problem is convex.

Value of  $p \in (1,2)$  suggests a compromise between the lasso and ridge regression. If p is closer to 1, the solver has the ability to put elements close to zero which is the nature of the lasso solver, If p is closer to 2, the solver more tends to shrink together correlated elements which is the nature of ridge regression.

Elastic-net, proposed by Zou and Hastie, introduced a different compromise between ridge and lasso [7]. The elastic-net selects the K largest elements like lasso, and shrinks the correlated elements together like ridge using a mixture penalty. The elastic net solver the problem given by

$$(P_{EN}): \ \widehat{\underline{X}}_{EN} = \arg\min_{\underline{X}} \|\underline{Y} - \mathbf{A}\underline{X}\|_{2}^{2} + \lambda \left(\alpha \|\underline{X}\|_{2}^{2} + (1 - \alpha)\|\underline{X}\|_{1}\right), \tag{20}$$

where  $\alpha$  is a mixing rate of the mixture penalty. We borrow Fig.6 from the book (Figure 3.13 of [1]). This figure compares contours of the  $L_p$  norm penalty with p=1.2 and the mixture penalty with  $\alpha=0.2$ . It is very difficult to distinguish those two penalties by eyes. Although those two are visually very similar, there exists a fundamental difference. The elastic-net has sharp (non-differentiable) corners such that it

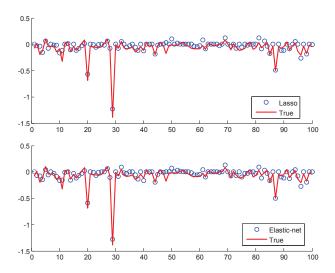


Fig. 7. Correlated signal estimation via lasso (Upper plot), and via the elastic-net (bottom plot) where N=100, K=3 and correlation coefficient  $\rho=0.5$  where the MSE of lasso estimate is 0.1136, while that of the elastin-net is 0.0801 in this example.

can put the elements exactly zero, whereas the  $L_p$  penalty does not [7]. Likewise with lasso, the elasticnet can be solved via quadratic programming, and the *LARs-EN* algorithm was introduced as a LARs type algorithm to solve the elastic-net problem by Zou and Hastie [7]

We compare the elastic-net solver to the lasso solver in Fig.7. For the comparison, we test a signal consisting of the K largest correlated elements and N-K small correlated elements where N=100, K=3, and the correlation coefficient  $\rho=0.5$ . We set the elastic-net parameters  $\alpha=0.4$ , and we use  $\lambda=0.001$  for the lasso and elastic-net both. In Fig.7, the elastic-net with appropriately calibrated parameters  $\alpha, \lambda$  surely improves the estimation accuracy from lasso although it is very hard to be distinguished by eyes. Indeed, the MSE of lasso estimate is 0.1136, while that of the elastin-net is 0.0801 in this example.

## B. Fused Lasso for Piecewise Smooth Signals

The use of various types of penalties enables us to solve the  $\underline{Y} = \mathbf{A}\underline{X}$  problem adaptively to the characteristic of the signal  $\underline{X}$ . The *fused lasso* is one of such solvers to find piecewise smooth signals. The fused lasso solves the problem given by

$$(P_{FL}): \ \widehat{\underline{X}}_{FL} = \arg\min_{\underline{X}} \|\underline{Y} - \mathbf{A}\underline{X}\|_{2}^{2}$$

$$+ \lambda \left(\alpha \sum_{i=2}^{N} |X_{i} - X_{i-1}| + (1 - \alpha) \|\underline{X}\|_{1}\right), \tag{21}$$

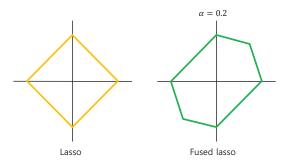


Fig. 8. Contours of the Lasso penalty (left plot) and the fuse lasso penalty ( $\alpha = 0.2$ ) (right plot)

where the difference penalty,  $\sum_{i=2}^{N} |X_i - X_{i-1}|$ , enforces the estimate  $\widehat{\underline{X}}_{FL}$  to be piecewise smooth by considering the order of the features. Namely, the fuse lasso encourages both sparsity of the signal values and sparsity of difference between adjacent elements. Fig.8 shows contour plot of the fused lasso penalty compared to that of the lasso penalty. As shown in Fig.8, the fused lasso penalty has asymmetric contour owing the difference penalty, and it becomes severe as  $\alpha$  increases. This asymmetricity of the fused lasso encourages the smoothness of the signal.

We show an example of the piecewise smooth signal recovery using a fused lasso solver in Fig.9, where measurements  $\underline{Y}$  is generated from a piecewise smooth signal  $\underline{X}$  with N=100, M=50 using a standard Gaussian matrix  $\mathbf{A}$ . This example shows that the piecewise smooth signal can be recovered via the fused lasso as  $\alpha$  increases although the signal  $\underline{X}$  itself is not sparse. We also checked that the signal can be recovered even from M=25 measurements when  $\alpha=0.9$ . In the figure, the case of  $\alpha=0$  is noteworthy because the case is equivalent to the conventional lasso case. This case informs us that such a piecewise smooth recovery is not successful via the normal lasso solver.

# V. CONCLUSIVE REMARKS

We have discussed about shrinkage method to solve the linear system  $\underline{Y} = \mathbf{A}\underline{X}$ . Estimation through such a method has smaller MSE than LSE at the expense of losing the unbiasedness. Ridge regression is one of the shrinkage methods applying a penalty on the energy of  $\underline{X}$ . This ridge penalty makes the solver to shrinks the correlated elements of  $\underline{X}$  together. Estimation accuracy of ridge is not satisfied for the K sparse signal estimation because the ridge solver cannot exactly fit the nonzero elements of  $\underline{X}$ . We also have introduced the lasso solver which imposes  $L_1$ -norm penalty of  $\underline{X}$ . The lasso solver shrinks the elements of  $\underline{X}$  according to their magnitude, performing the shrinkage as a soft thresholding function. The estimation accuracy of lasso is very good for K sparse signals by putting the nonzero elements of  $\underline{X}$ 

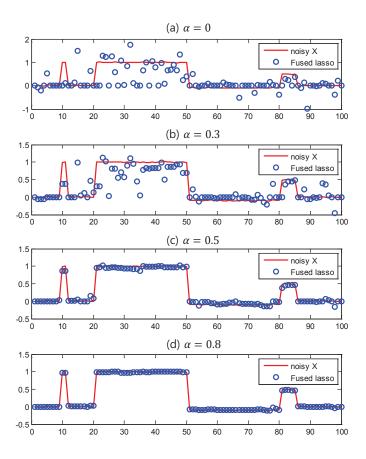


Fig. 9. Piecewise smooth signal estimation via fused lasso for a variety of  $\alpha$  when  $N=100, M=50, \lambda=0.01$ 

exactly to zero. Elastic-net solver is a compromise of ridge and lasso using a mixture penalty. This solver has ability to put the nonzero element to zero as well as, to shrink the correlated element together. The fused lasso solver was devised to find piecewise smooth signals. Imposing of difference penalty which reflect the order of signal features enables us to estimate the piecewise smooth signal effectively.

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