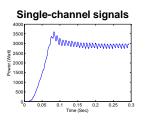
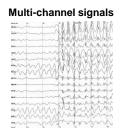
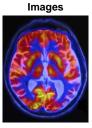


Sparse Information and Regularization

- High-dimensional data usually have a low dimensional structure.
- Important information of HD data is embedded in a few dimensions (sparse) and the rest are non-informative and noise





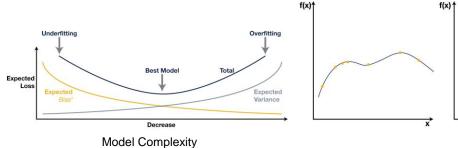




 Regularization helps identify the spares informative features and remove the noise.

Model Complexity and Regularization

Regularization can help adjust model complexity to avoid overfitting.



General Form of Regularization

 Typically a regularized estimation is performed by solving the following optimization problem:

$$\min\{L(\theta; Z_i) + \lambda P(\theta)\}\$$

- $L(\theta; Z_i)$ is a loss function (or negative likelihood function)
- $P(\theta)$ is a penalty function.
- λ adjusts the level of regularization.
- Examples include Ridge, Lasso, Non-negative Garrote, Adaptive Lasso, Group Lasso, etc.

$$\min_{\beta_{i}} \sum_{i=1}^{n} \left(y_{i} - \sum_{j=1}^{p} \beta_{j} x_{ij} \right)^{2} + \lambda \sum_{j=1}^{p} \beta_{j}^{2}$$

Ridge Regression

Assuming the observations are centered, Ridge estimates can be computed by

$$\min_{\beta_{i}} \sum_{i=1}^{n} \left(y_{i} - \sum_{j=1}^{p} \beta_{j} x_{ij} \right)^{2} + \lambda \sum_{j=1}^{p} \beta_{j}^{2}$$

The Ridge objective function in a matrix form is

$$\min_{\boldsymbol{\beta}} \left\| \boldsymbol{y} - \boldsymbol{X} \boldsymbol{\beta} \right\|_2^2 + \lambda \left\| \boldsymbol{\beta} \right\|_2^2$$

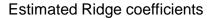
$$\hat{\boldsymbol{\beta}}^{ridge} = (\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_p)^{-1} \mathbf{X}^T \mathbf{y}$$

- Estimated Ridge coefficients are shrunken towards zero
- λ≥0 is the tuning parameter controls the amount of shrinkage
- λ is chosen based on some prediction criteria (MSE) using CV or independent validation data set

Ridge Regression

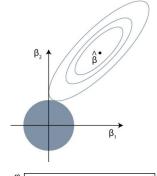
An equivalent formulation is given by

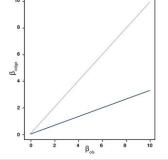
$$\min_{\beta_i} \sum_{i=1}^n \left(y_i - \sum_{j=1}^p \beta_j x_{ij} \right)^2$$
subject to
$$\sum_{i=1}^p \beta_j^2 \le s$$



- Are linear in y
- Are biased
- Have smaller variance

$$\hat{\boldsymbol{\beta}}^{ridge} = \left(\mathbf{X}^T \mathbf{X} + \lambda \mathbf{I}_p \right)^{-1} \mathbf{X}^T \mathbf{y}$$

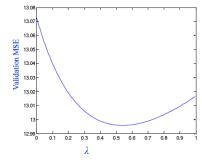


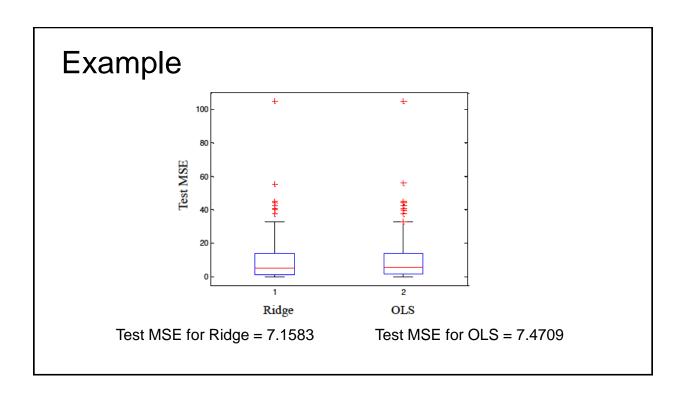


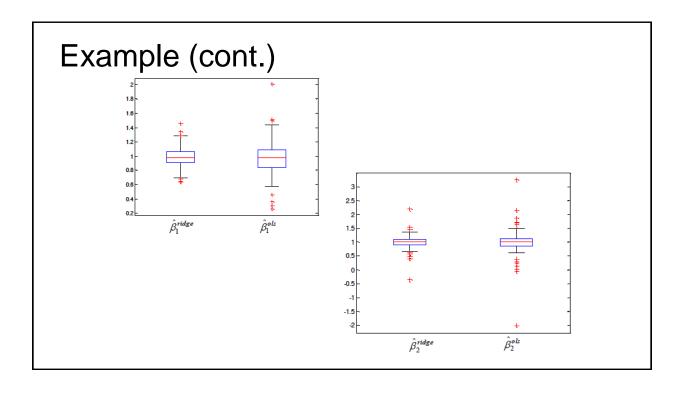
Example

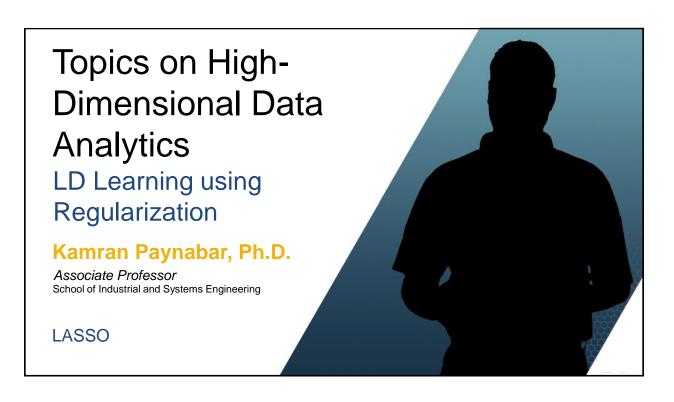
- A sample of 100 centered training data including one response and two independent variables is simulated. $y_i = x_{i1} + x_{i2} + \varepsilon_i$; $\varepsilon_i \sim N(0,0.5)$
- Two other independent samples are simulated for validation and test
- Both OLS and Ridge Regression are applied to estimate regression coefficients
- This procedure is repeated 100 times

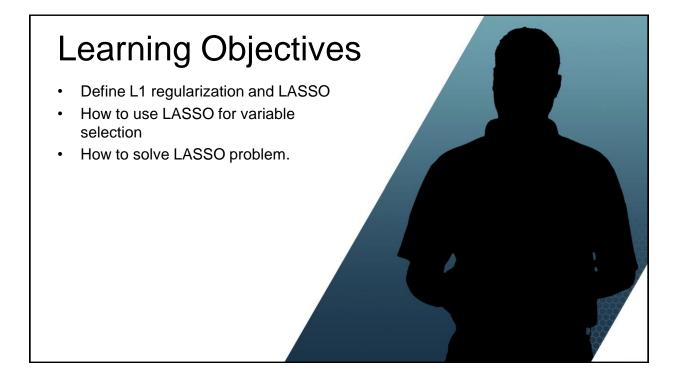
$$\min_{\beta_j} \sum_{i=1}^n \left(y_i - \sum_{j=1}^p \beta_j x_{ij} \right)^2 + \lambda \sum_{j=1}^p \beta_j^2$$











Variable (Feature) Selection

To determine a smaller subset of predictors that exhibit the strongest correlation with response. Traditional variable selection methods include:

- Forward selection
- · Backward elimination
- · Stepwise selection

The selection process is discrete and thus unstable.

Variable (Feature) Selection using Regularization

- Regularized regression provides with a more stable variable selection procedure compared with traditional variable selection methods.
- If an estimated coefficient for a predictor is zero then the predictor may not have information about the response variable.
- Ridge regression can control model complexity by reducing the variance.
- However, the L2 norm or ridge regression cannot be used for variable selection. That is the solution to the ridge problem is likely non-zero.
- L0 and L1 norm, however, can provide sparse solutions where most of noninformative variables have coefficients equal to zero.

Variable Selection Using L₀ Norm

Suppose we know that the number of non-zero coefficients is at most K. Then using L_0 a regularized (penalized) OLS can be written as

$$\hat{\beta} = \operatorname{argmin} \|y - X\beta\|_2^2$$
$$\|\beta\|_0 \le K$$

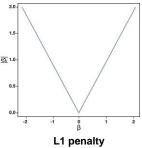
- *L*₀ norm is the total number of nonzero elements in a vector.
- This problem is combinatorial. The best subset selection approach can be used to solve it.
- Since this approach requires solving an OLS for all possible subsets, it is not efficient for cases with a large number of predictors.
- An alternative solution is find an appropriate convex approximation by replacing L_0 norm with L_1 norm.

LASSO: Least Absolute Shrinkage and Selection Operator

Assuming the observations are centered, lasso estimates can be computed by (Chen, Donoho and Saunders 1996; Tibshirani 1996)

$$\hat{\beta} = \operatorname{argmin} \|y - X\beta\|_2^2$$
 Equivalently $\hat{\beta} = \operatorname{argmin} \|y - X\beta\|_2^2 + \lambda \|\beta\|_1$

- Shrinkage: estimated lasso coefficients are shrunken towards zero
- Sparsity: some fitted coefficients are exactly zero
- Continuous variable selection
- λ≥0 is the tuning parameter controls the amount of sparsity



LASSO

$$\min_{\beta_i} \sum_{i=1}^n \left(y_i - \sum_{j=1}^p \beta_j x_{ij} \right)^2$$
 subject to
$$\sum_{j=1}^p \left| \beta_j \right| \le s$$

$$\max_{\beta_i} \sum_{j=1}^n \left(y_i - \sum_{j=1}^p \beta_j x_{ij} \right)^2$$
 Ridge

LASSO with Orthonormal Predictors

$$\min_{\beta_j} \sum_{i=1}^n \left(y_i - \sum_{j=1}^p \beta_j x_{ij} \right)^2 + \lambda \sum_{j=1}^p \left| \beta_j \right|$$

When X is orthonormal the above minimization model is reduced to

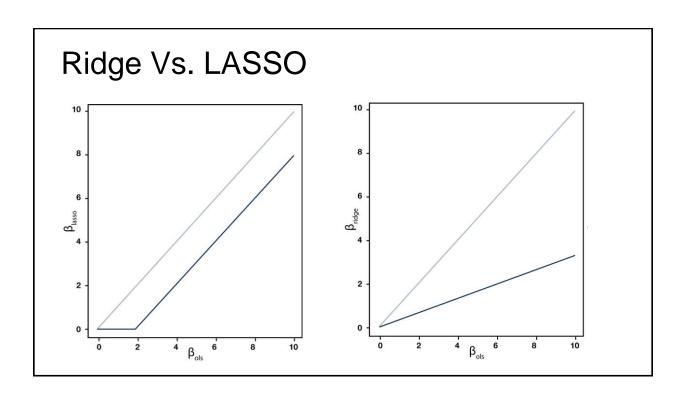
$$\min_{\beta_{j}} \left(\beta_{j} - \hat{\beta}_{j}^{ols} \right)^{2} + \lambda \left| \beta_{j} \right|$$

The closed-from solution is given by

$$\hat{\beta}_{j}^{\text{lasso}} = \begin{cases} \hat{\beta}_{j}^{\text{ols}} - \frac{\lambda}{2} & \text{if } \hat{\beta}_{j}^{\text{ols}} > \frac{\lambda}{2} \\ 0 & \text{if } |\hat{\beta}_{j}^{\text{ols}}| \leq \frac{\lambda}{2} \\ \hat{\beta}_{j}^{\text{ols}} + \frac{\lambda}{2} & \text{if } \hat{\beta}_{j}^{\text{ols}} < -\frac{\lambda}{2} \end{cases}$$

$$= \operatorname{sign}(\hat{\beta}_{j}^{\text{ols}}) \cdot \left(|\hat{\beta}_{j}^{\text{ols}}| - \frac{\lambda}{2} \right)$$

 Lasso shrinks large coefficients by a constant. Lasso truncates small coefficients to zero.

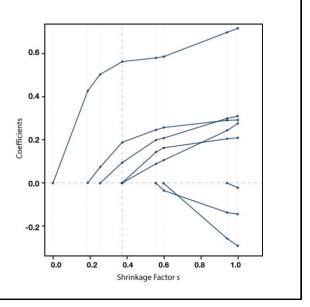


Computation

Convex optimization: Lasso can be solved using convex programming

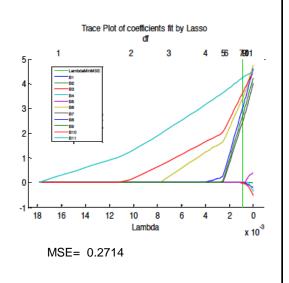
Piecewise linear solution path by LARS: (Efron et al., 2004)

- The path of solution is piecewise linear in λ
- Cost is approximately one leastsquare calculation



For a regression setting with a 11 predictors, 100 observations are generated such that 5 predictors are not informative.

- Lasso is used to identify important variables and fit a prediction model.
- A 10-fold cross validation is used to choose the tuning parameter.



Example

clear all load predictors

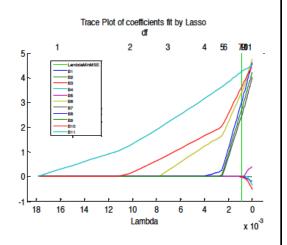
end

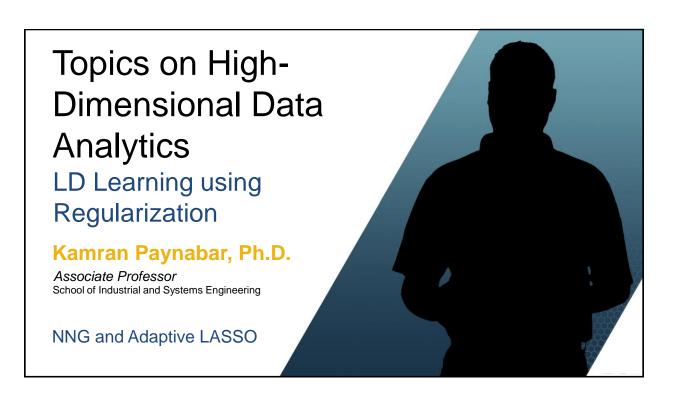
for i=1:100 T(i)=X(i,:)*[0 0 0 0 0 4*ones(1,6)]'+normrnd(0,0.5);

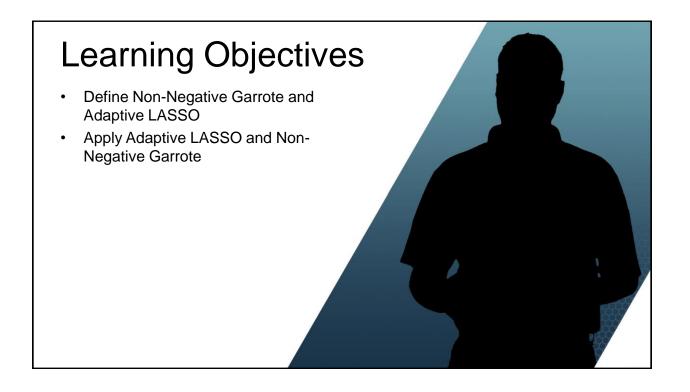
[B,FitInfo] = lasso(X,T,'CV',10,'Standardize', 0, 'Alpha',1) ax = lassoPlot(B,FitInfo, 'PlotType', 'Lambda')

B(:,FitInfo.IndexMinMSE)

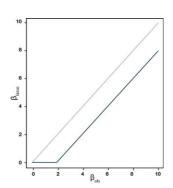
FitInfo.MSE(FitInfo.IndexMinMSE)

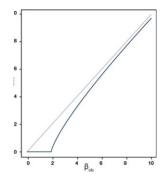






Constant Shrinkage in Lasso





- · Lasso shrinks all large coefficients by a constant;
- · A better shrinkage would consider the magnitude of coefficients in shrinkage;
- · Lasso is not consistent in variable selection.

Non-Negative Garrote

Consider lasso with the following change of variables

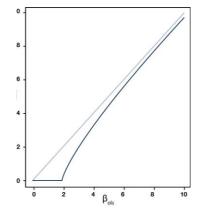
$$\min_{d_j} \sum_{i=1}^n \left(y_i - \sum_{j=1}^p d_j \hat{\beta}_j^{ols} x_{ij} \right)^2 + \lambda \sum_{j=1}^p d_j$$
subject to $d_j \ge 0$



$$\hat{\boldsymbol{\beta}}_{i} = \hat{d}_{i} \hat{\boldsymbol{\beta}}_{i}^{ols}$$

- NNG is proposed by Breiman (1995)
- Closed-form solution in orthonormal case

$$\hat{\beta}_{j}^{\text{garrote}} = \text{sign}(\hat{\beta}_{j}^{\text{ols}}) \cdot \left(|\hat{\beta}_{j}^{\text{ols}}| - \frac{1}{2} \frac{\lambda}{|\hat{\beta}_{j}^{\text{ols}}|} \right)_{+}$$



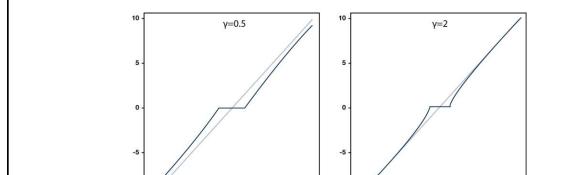
Adaptive LASSO

Adaptive LASSO

Assuming the observations are centered, adaptive lasso estimates can be computed by

$$\beta^{\text{Alasso}} = \operatorname{argmin} \|y - X\beta\|_2^2 + \lambda_n \sum_{j=1}^p \widehat{w}_j |\beta_j|$$

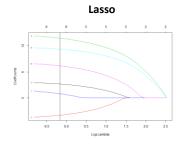
- where \widehat{w}_j is a weight defined by $\widehat{w}_j = \frac{1}{\left|\widehat{\beta}_j^{ols}\right|^{\gamma}}$, $\widehat{w}_j = \frac{1}{\left|\widehat{\beta}_j^{ridge}\right|^{\gamma}}$, etc.
- Adaptive lasso (Zou, 2007) is very similar to NNG.

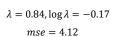


$$\beta^{\text{Alasso}} = \min \|y - X\beta\|_2^2 + \lambda_n \sum_{j=1}^p \widehat{w}_j |\beta_j|$$

True model

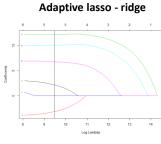
$$\begin{aligned} y_i &= 6.94x_3 - 4.03x_6 + 1.90x_{11} + 3.23x_{14} + 12.26x_{18} + 9.99x_{20} + \epsilon_i \\ y &\in \mathbb{R}^{100}, X \in \mathbb{R}^{100 \times 20}, \epsilon \in \mathbb{R}^{100} \end{aligned}$$





Adaptive lasso - ols

$$\lambda = 499,558.56 \log \lambda = 13.12$$
 $mse = 3.19$



$$\gamma = 2$$
 $\lambda = 12,892.95, \log \lambda = 9.46$
 $mse = 4.73$

Example

True model

$$\begin{aligned} y_i &= -8.18x_1 + 4.17x_2 + 9.23x_5 + 3.90x_8 + 8.56x_{10} + 7.40x_{14} + \epsilon_i \\ y &\in \mathbb{R}^{100}, X \in \mathbb{R}^{100 \times 20}, \epsilon \in \mathbb{R}^{100} \end{aligned}$$

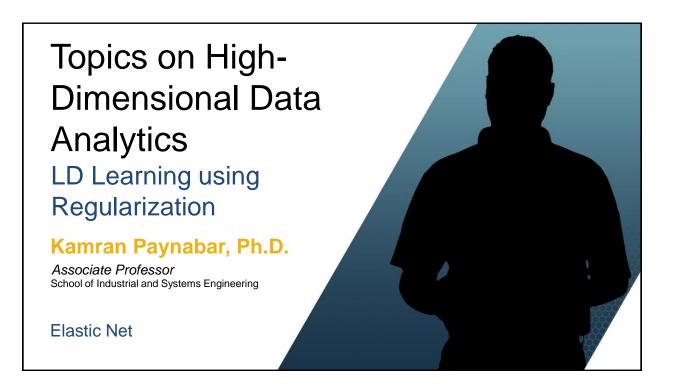
Using CV, to find the optimal lambda we get:

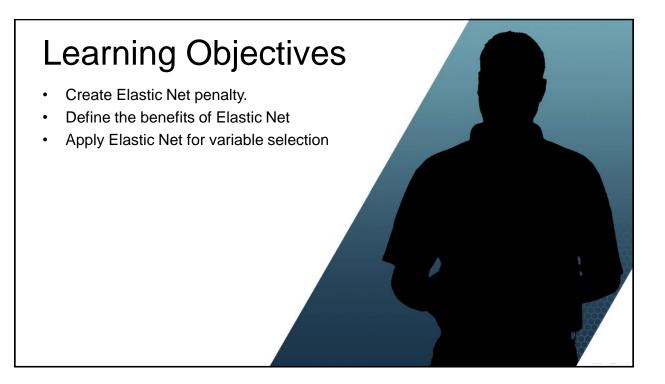
	True beta	Lasso	Alasso - ols	Alasso - ridge
3	6.94	6.45	6.90	6.91
6	-4.03	-3.47	-3.73	-3.76
11	1.90	1.33	0.93	1.00
14	3.23	2.61	2.73	2.76
18	12.26	11.72	12.22	12.23
20	9.99	9.38	9.93	9.93

Data generation

p = 20 #Number of parameters
n = 100 #Number of observaations
x = rnorm(p*n,0,1)
X = matrix(x,nrow = n)
rm(x)
n0 = sample(1:p,6)
beta = rep(0,p)
beta[n0] = rnorm(6,0,5)
y = X%**%beta + rnorm(n,0,0.5)

```
# Lasso
lasso = cv.glmnet(X, y, family = "gaussian", alpha = 1, intercept = FALSE)
lambda = lasso$lambda.min
coef.lasso = matrix(coef(lasso, s = lambda))[2:(p+1)]
lasso = glmnet(X, y, family = "gaussian", alpha = 1, intercept = FALSE)
plot(lasso, xvar = "lambda", label = TRUE, main = "Lasso")
abline(v = log(lambda))
# Adaptive lasso
gamma = 2
b.ols = solve(t(X)\%*\%X)\%*\%t(X)\%*\%y
ridge = cv.glmnet(X, y, family = "gaussian", alpha = 0, intercept = FALSE)
I.ridge = ridge$lambda.min
b.ridge = matrix(coef(ridge, s = l.ridge))[2:(p+1)]
w1 = 1/abs(b.ols)^gamma
w2 = 1/abs(b.ridge)^gamma
alasso1 = cv.glmnet(X, y, family = "gaussian", alpha = 1, intercept = FALSE, penalty.factor = w1)
alasso2 = cv.glmnet(X, y, family = "gaussian", alpha = 1, intercept = FALSE, penalty.factor = w2)
lambda1 = alasso1$lambda.min
lambda2 = alasso2$lambda.min
coef.alasso1 = matrix(coef(alasso1, s = lambda1))[2:(p+1)]
coef.alasso2 = matrix(coef(alasso2, s = lambda2))[2:(p+1)]
alasso1 = glmnet(X, y, family = "gaussian", alpha = 1, intercept = FALSE, penalty.factor = w1)
alasso2 = glmnet(X, y, family = "gaussian", alpha = 1, intercept = FALSE, penalty.factor = w2)
plot(alasso1, xvar = "lambda", label = TRUE, main = "Adaptive lassso - ols")
abline(v=log(lambda1))
plot(alasso2, xvar = "lambda", label = TRUE, main = "Adaptive lassso - ridge")
abline(v=log(lambda2))
```





Elastic Net

Assuming the observations are centered, Elastic Net estimates can be computed by (Zou and Hastie, 2006)

$$\min_{\boldsymbol{\beta}} \left\| \mathbf{y} - \mathbf{X} \boldsymbol{\beta} \right\|_2^2 + \lambda_1 \left\| \boldsymbol{\beta} \right\|_1 + \lambda_2 \left\| \boldsymbol{\beta} \right\|_2^2$$

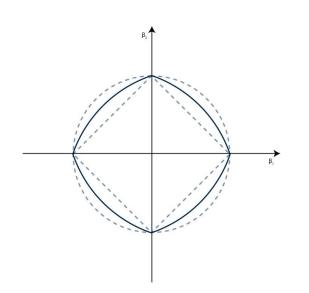
- L1 penalty: encourages sparsity
- · L2 penalty:
 - Helps perform variable selection when important variable is more than n
 - Alleviates the drawback of multicolinearity

Given λ_2 the solution path of elastic net coefficients is piecewise linear in λ_1

$$\mathbf{X}_{(n+p)\times p}^* = (1+\lambda_2)^{-\frac{1}{2}} \begin{pmatrix} \mathbf{X} \\ \sqrt{\lambda_2} \mathbf{I} \end{pmatrix}, \quad \mathbf{y}_{(n+p)}^* = \begin{pmatrix} \mathbf{y} \\ 0 \end{pmatrix}$$

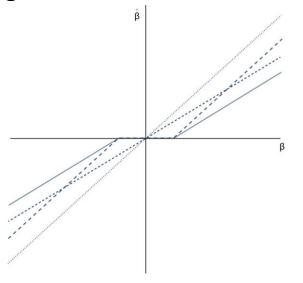
Elastic Net

$$\min_{\beta_{j}} \sum_{i=1}^{n} \left(y_{i} - \sum_{j=1}^{p} \beta_{j} x_{ij} \right)^{2}$$
subject to $\alpha \sum_{j=1}^{p} \left| \beta_{j} \right| + (1 - \alpha) \sum_{j=1}^{p} \beta_{j}^{2} \leq s$



Elastic Net Estimates

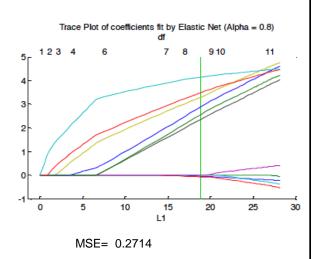
 $\min_{\boldsymbol{\beta}} \left\| \mathbf{y} - \mathbf{X} \boldsymbol{\beta} \right\|_{2}^{2} + \lambda_{1} \left\| \boldsymbol{\beta} \right\|_{1} + \lambda_{1} \left\| \boldsymbol{\beta} \right\|_{2}^{2}$



(Zou and Hastie, 2006)

For a regression setting with a 11 predictors, 100 observations are generated such that 5 predictors are not informative.

- Elastic Net is used to identify important variables and fit a prediction model.
- A 10-fold cross validation is used to choose the tuning parameter.



Example

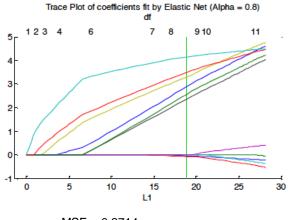
clear all load predictors

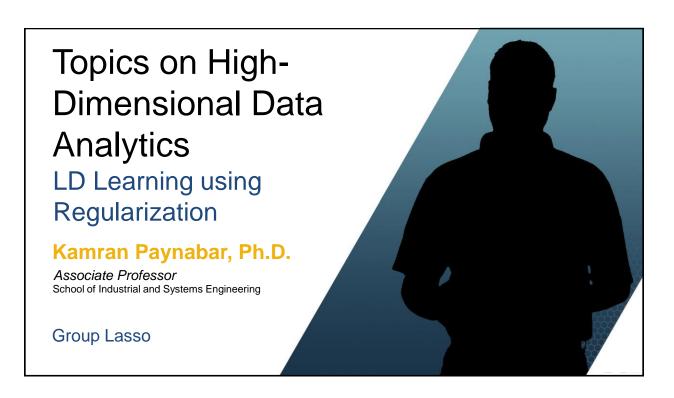
for i=1:100

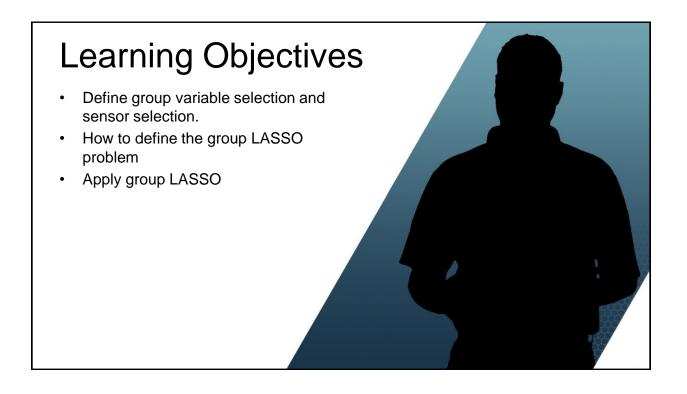
T(i)=X(i,:)*[0 0 0 0 0 4*ones(1,6)]'+normrnd(0,0.5); end

[B1,FitInfo1] = lasso(X,T,'CV',10,'Standardize', 0 , 'Alpha' ,0.8) ax1 = lassoPlot(B1,FitInfo1)

B1(:,FitInfo1.IndexMinMSE) FitInfo1.MSE(FitInfo1.IndexMinMSE)

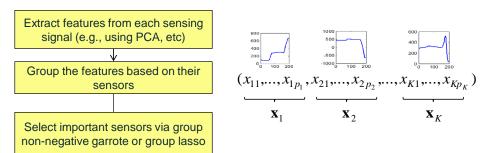






Group Variable Selection

- In some cases, features or variables are naturally partitioned into grouped variables, for example
 - Each factor in ANOVA is a group variable that includes dummy variables representing the levels of the factor.
 - The features extracted from a signal can form a grouped variable.



Group LASSO

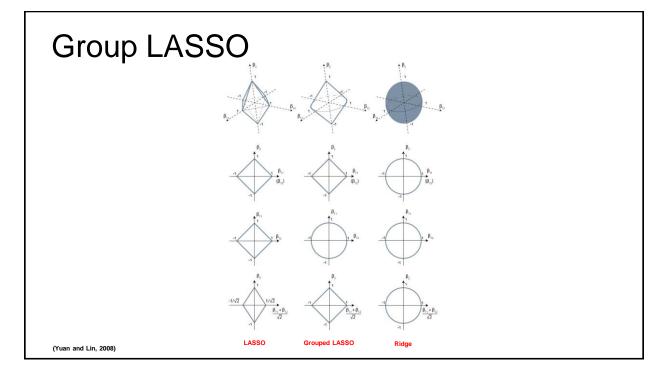
Assuming the observations are centered, group lasso estimates can be computed by (Yuan and Lin, 2008)

$$\min_{\hat{\boldsymbol{\beta}}_k} \frac{1}{2} \left\| \mathbf{y} - \sum_{k=1}^K \mathbf{X}_k \hat{\boldsymbol{\beta}}_k \right\|^2 + \lambda_1 \sum_{k=1}^K \left\| \boldsymbol{\beta}_k \right\|$$

where

$$\|\mathbf{\beta}_{k}\| = \sqrt{\sum_{j=1}^{p_{k}} \beta_{kj}^{2}}$$

$$(\underline{x_{11}, \dots, x_{1p_{1}}}, \underline{x_{21}, \dots, x_{2p_{2}}}, \dots, \underline{x_{K1}, \dots, x_{Kp_{K}}})$$



Other Group Variable Selection Methods

$$\min_{\hat{\boldsymbol{\beta}}_k} \frac{1}{2} \left\| \mathbf{y} - \sum_{k=1}^K \mathbf{X}_k \hat{\boldsymbol{\beta}}_k \right\|^2 + J(\lambda_t, \hat{\boldsymbol{\beta}}_k)$$

Group Lasso L₂ (Yuan and Lin, 2008)
$$J(\lambda_i, \beta_{kj}) = \lambda_1 \sum_{k=1}^{K} \|\mathbf{\beta}_k\|$$
 $\|\mathbf{\beta}_k\| = \sqrt{\sum_{j=1}^{P_k} \beta_{kj}^2}$

$$J(\lambda_t, \beta_{kj}) = \lambda_1 \sum_{k=1}^{K} \left\| \boldsymbol{\beta}_k \right\|$$

$$\|\boldsymbol{\beta}_k\| = \sqrt{\sum_{i=1}^{p_k} \beta_{kj}^2}$$

Group Lasso
$$L_{\infty}$$
 (Zhao et al., 2009)
$$J(\lambda_{i}, \beta_{kj}) = \lambda_{1} \sum_{k=1}^{K} \|\mathbf{\beta}_{k}\|_{\infty} \qquad \|\mathbf{\beta}_{k}\|_{\infty} = \max_{j} \left\{ \beta_{kj} \right\}$$

$$J(\lambda_{t}, \beta_{kj}) = \lambda_{1} \sum_{k=1}^{K} \| \boldsymbol{\beta}_{k} \|_{\infty}$$

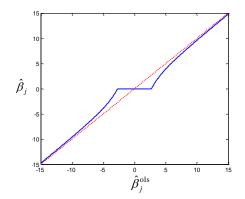
$$\left\| \boldsymbol{\beta}_{k} \right\|_{\infty} = \max_{j} \left\{ \beta_{kj} \right\}$$

$$J(\lambda_t, \beta_{kj}) = \lambda_1 \sum_{k=1}^{K} d_k \qquad \qquad \mathbf{\beta}_k = d_k \hat{\mathbf{\beta}}_k^{\text{ols}}; d_k \ge 0$$

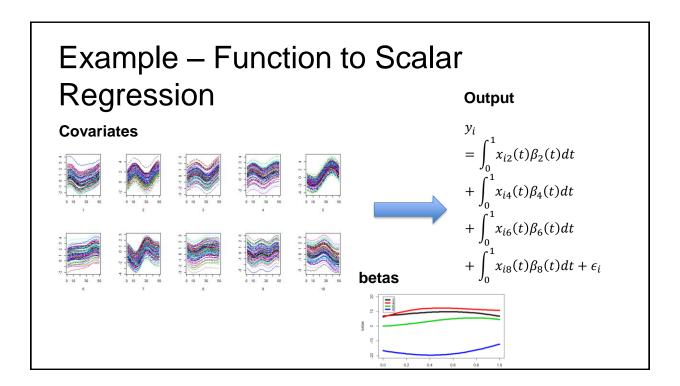
$$\boldsymbol{\beta}_k = d_k \hat{\boldsymbol{\beta}}_k^{\text{ols}}; d_k \ge 0$$

Group NNG: Orthogonal Basis Case

In case of orthogonal predictors (e.g., wavelets) there is a closed-form solution in form of soft-thresholding estimates



$$\hat{d}_k = \left(1 - \lambda / \sum_{j=1}^{p_k} (\hat{\beta}_{kj}^{\text{ols}})^2\right)$$



Example – Function to Scalar Regression

$$y_i = \sum\nolimits_{j = 1}^{10} {\int\nolimits_0^1 {{x_{ij}}(t)\beta _j(t)dt} } + \epsilon_i$$

We can use b-splines to reduce the dimensionality:

$$\beta_j(t) = \sum_{k=1}^{10} b_{kj} \theta_{kj}(t) = \boldsymbol{\theta}_j^T \boldsymbol{b}_j$$

With this, we have:

$$\int_0^1 x_{ij}(t)\beta_j(t)dt = \int_0^1 x_{ij}(t)\boldsymbol{\theta_j}^T(t)dt\boldsymbol{b_j} = \boldsymbol{z_{ij}b_j}$$

Therefore:

$$y_i = z_{i1}b_1 + z_{i2}b_2 + \dots + z_{i10}b_{10} + \epsilon_i$$

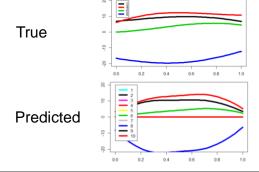
 $y_i = z_{i1}b_1 + z_{i2}b_2 + \dots + z_{i10}b_{10} + \epsilon_i$ Our goal is to estimate $b_j \in \mathbb{R}^{10 \times 1}$, using group lasso. The problem we want to solve is:

$$\min_{\boldsymbol{b}} \left| |\boldsymbol{y} - \boldsymbol{Z}\boldsymbol{b}| \right|_{2}^{2} + \sum_{j=1}^{10} \left| |\boldsymbol{b}_{j}| \right|_{2}$$

Example – Function to Scalar Regression

$$y_i = \sum_{j=1}^{10} \int_0^1 x_{ij}(t) \beta_j(t) dt + \epsilon_i$$

Prediction using group lasso:



Learned B-spline coefficients:

	b1	b2	b3	b4	b5	b6	b7	b8	b9	b10
coef1	0.00	3.43	0.00	3.44	0.00	0.45	0.00	-8.13	0.00	0.00
coef2	0.00	5.05	0.00	5.44	0.00	0.86	0.00	-12.04	0.00	0.00
coef3	0.01	7.78	0.00	8.61	0.00	1.67	0.00	-17.60	0.00	0.00
coef4	0.01	10.52	0.00	12.10	0.00	2.90	0.00	-22.73	0.00	0.00
coef5	0.01	10.50	0.00	12.90	0.00	3.77	0.00	-21.90	0.00	0.00
coef6	0.01	10.53	0.00	13.71	0.00	4.67	0.00	-20.91	0.00	0.00
coef7	0.01	10.71	0.00	14.61	0.00	5.57	0.00	-20.08	0.00	0.00
coef8	0.01	8.01	0.00	11.45	0.00	4.72	0.00	-14.74	0.00	0.00
coef9	0.01	5.23	0.00	7.78	0.00	3.40	0.00	-9.71	0.00	0.00
coef10	0.00	3.48	0.00	5.24	0.00	2.40	0.00	-6.30	0.00	0.00

Example – Function to Scalar Regression

Data generation

 $\begin{array}{ll} p=10 & \text{\#Number of parameters} \\ tp=4 & \text{\#Number of true parameters} \\ n=50 & \text{\#Length of observations} \\ m=100 & \text{\#Number of observations} \\ snr=200 \\ ds=0.2 \end{array}$

x_1 = list()

```
for(i in 1:p)
\{x = seq(0,1,length=n)\}
 E = as.matrix(dist(x, diag=T, upper=T))
 Sigma = exp(-10*E^2)
 eig = eigen(Sigma)
 Sigma.sqrt = eig\$vec\%*\%diag(sqrt(eig\$val+10^{-10}))\%*\%t(eig\$vec)
 mean1 = Sigma.sqrt%*%rnorm(n)
 S_noise = exp(-0.1*E^2)
 eig_noise = eigen(S_noise)
 S.sqrt_noise = eig_noise$vec%*%diag(sqrt(eig_noise$val+10^(-10)))%*%t(eig_noise$vec)
 noise = S.sqrt_noise%*%rnorm(n)
 signal = mean1 + noise
 var = var(signal)
 ds1 = sqrt(var/snr)
 S.sqrt\_err = diag(n)*drop(ds1)
 x1 = matrix(0,m,n)
 for(j in 1:(m)) {
  noise = S.sqrt_noise%*%rnorm(n)
  error = S.sqrt_err%*%rnorm(n)
  x1[j,] = mean1 + noise + error }
 x_1[[i]] = x1
```