Biostatistics-Lecture 16 Model Selection

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- Interested in factors related to the life expectancy (50 US states, 1969-71)
 - Per capita income (1974)
 - Illiteracy (1970, percent of population)
 - Murder rate per 100,000 population
 - Percent high-school graduates
 - Mean number of days with min temperature < 30 degree
 - Land area in square mile

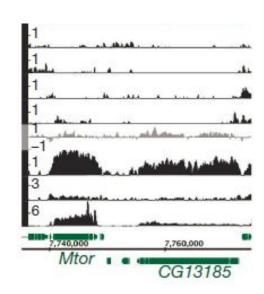
- The role of microRNA on regulating gene expression
 - Response: standard deviation of a gene expression
 - Covariates:
 - mean gene expression
 - length of the 3'-UTRs
 - number of microRNA targets in the 3'-UTRs
 - mean target score of the microRNA targets
 - number of common SNPs in the 3'-UTR
 - mean of minor allele frequencies of common SNPs in 3'-UTRs

	Expressio n SD	Expression Mean	Gene Length	Length of 3' UTR	Number of miRNA targets	Mean target score	Number of SNPs	Mean MAF
Expression								
SD	1	0.952031	0.084030	0.068084	0.146080	0.135781	0.035820	0.033893
Expression								
Mean	0.952031	1	0.157620	0.120004	0.165147	0.156963	0.055338	0.051066
Gene Length	0.084030	0.157620	1	0.471435	0.406605	0.311641	0.216913	0.173899
Length of 3'								
UTR	0.068084	0.120004	0.471435	1	0.246593	0.206723	0.227899	0.197424
Number of miRNA								
targets	0.146080	0.165147	0.406605	0.246593	1	0.849602	0.185446	0.142214
Mean target								
score	0.135781	0.156963	0.311641	0.206723	0.849602	1	0.151916	0.128167
Number of								
SNPs	0.035820	0.055338	0.216913	0.227899	0.185446	0.151916	1	0.947236
Mean MAF	0.033893	0.051066	0.173899	0.197424	0.142214	0.128167	0.947236	1

- Communities and Crime
 - Response: total number of violent crimes per 100K population
 - Covariates (128):
 - population for community
 - percentage of population that is caucasian
 - percentage of population that is african american
 - median household income
 - per capita income for african americans
 - percentage of kids born to never married
 - number of vacant households
 - number of sworn full time police officers
 -
 - http://archive.ics.uci.edu/ml/datasets/Communities+and+Crime

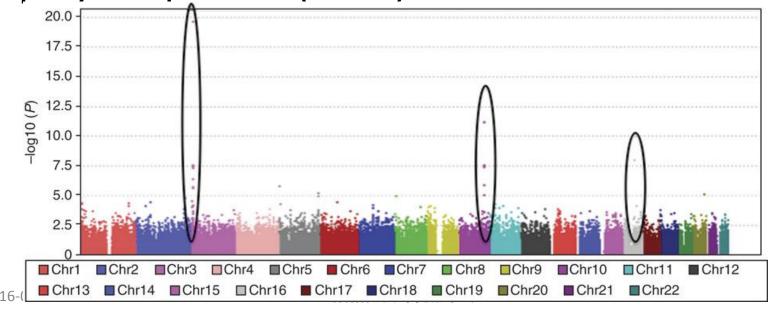
Motif finding





- Response: univariate response measuring binding intensity (ChIP-seq or ChIP-chip data)
- Covariates (~200): abundant score of candidate motifs

- Genome-wide association studies
- Response: disease or not
- Covariates (~10⁶): single nucleotide polymorphisms (SNPs)



- Expression quantitative trait loci (eQTL) studies
 - Response (~ 20,000): gene expression
 - Covariates(~10⁶): SNPs

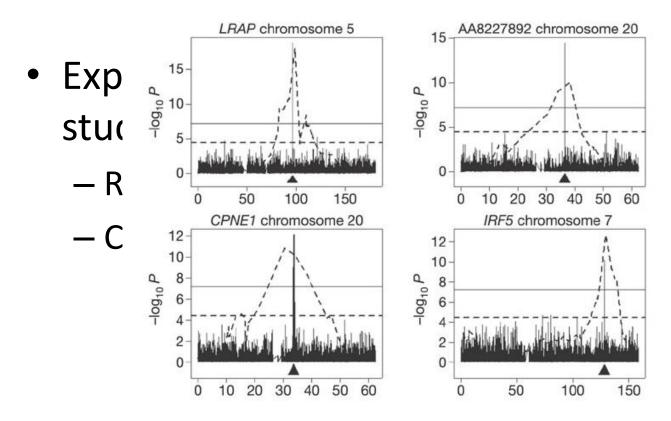


Figure 17: Figure adopted from Cheung et al. Figure 1

General framework

general framework:

$$Z_1, \ldots, Z_n$$
 (with some "i.i.d. components") $\dim(Z_i) \gg n$

for example:

$$Z_i = (X_i, Y_i), \ X_i \in \mathcal{X} \subseteq \mathbb{R}^p, Y_i \in \mathcal{Y} \subseteq \in \mathbb{R}$$
: regression with $p \gg n$ $Z_i = (X_i, Y_i), \ X_i \in \mathcal{X} \subseteq \mathbb{R}^p, Y_i \in \{0, 1\}$: classification for $p \gg n$

General framework

$$Y_{i} = \sum_{j=1}^{p} \beta_{j}^{0} X_{i}^{(j)} + \varepsilon_{i}, i = 1, ..., n$$

$$p \gg n$$
in short: $\mathbf{Y} = \mathbf{X}\beta + \varepsilon$

goals:

- prediction, e.g. w.r.t. squared prediction error
- estimation of β^0 , e.g. w.r.t. $\|\hat{\beta} \beta^0\|_q$ (q = 1, 2)

Stepwise selection

Backward Elimination

- 1. Start with all the predictors in the model
- 2. Remove the predictor with highest p-value greater than α_{crit}
- 3. Refit the model and goto 2
- 4. Stop when all p-values are less than α_{crit} .

Stepwise selection

Forward Selection

- 1. Start with no variables in the model.
- 2. For all predictors not in the model, check their p-value if they are added to the model. Choose the one with lowest p-value less than α_{crit} .
- 3. Continue until no new predictors can be added.

Drawbacks of stepwise selection

- One-at-a-time: may miss optimal
- P-values of the remaining predictors tends to be overstated
 - Multiple testing
- Model tends to be smaller than desirable for prediction purpose
- Variable not in the model may still be correlated with the response

Stepwise selection—An example

- Interested in factors related to the life expectancy (50 US states, 1969-71)
 - Per capita income (1974)
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Bias, Variance, and Model Complexity

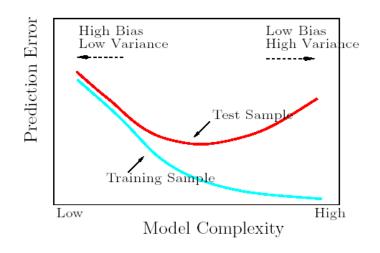


Figure 7.1: Behavior of test sample and training sample error as the model complexity is varied.

- Bias-Variance trade-off again
- Generalization: test sample vs. training sample performance
 - Training data usually monotonically increasing performance with model complexity

Measuring Performance

- ullet target variable Y
- Vector of inputs X
- Prediction model $\hat{f}(X)$
- Typical Choices of Loss function

$$L(Y, \hat{f}(X)) = \begin{cases} \left(Y - \hat{f}(X)\right)^{2} & squared \ error \\ \left|Y - \hat{f}(X)\right| & absolute \ error \end{cases}$$

Generalization Error

Test error. Generalization error

$$Err = E\left[L(Y, \hat{f}(X))\right]$$

- Note: This expectation averages anything that is random, including the randomness in the training sample that it produced
- Training error

$$\overline{err} = \frac{1}{N} \sum_{i=1}^{n} L(y_i, \hat{f}(x_i))$$

- average loss over training sample
- not a good estimate of test error (next slide)

Training Error

- Training error Overfitting
 - not a good estimate of test error
 - consistently decreases with model complexity
 - drops to zero with high enough complexity

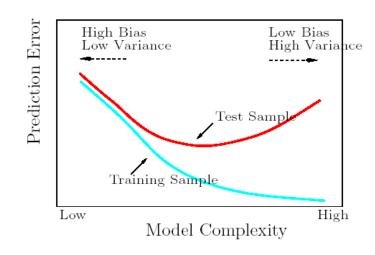


Figure 7.1: Behavior of test sample and training sample error as the model complexity is varied.

Two separate goals

- Model selection:
 - Estimating the performance of different models in order to choose the (approximate) best one
- Model assessment:
 - Having chosen a final model, estimating its prediction error (generalization error) on new data
- Ideal situation: split data into the 3 parts for training, validation (est. prediction error+select model), and testing (assess model)
- Typical split: 50% / 25% / 25%

Bias-Variance Decomposition

$$Y = f(X) + \varepsilon$$
, $E(\varepsilon) = 0$, $Var(\varepsilon) = \sigma_{\varepsilon}^{2}$

• Then for an input point $X = x_0$ using unit-square loss and regression fit:

$$\operatorname{Err}(x_0) = E[(Y - \hat{f}(x_0))^2 | X = x_0]$$

$$= \sigma_{\varepsilon}^2 + [\operatorname{E}\hat{f}(x_0) - f(x_0)]^2 + E[\hat{f}(x_0) - \operatorname{E}\hat{f}(x_0)]^2$$

$$= \sigma_{\varepsilon}^2 + \operatorname{Bias}^2(\hat{f}(x_0)) + \operatorname{Var}(\hat{f}(x_0))$$

$$= \operatorname{Irreducible} \operatorname{Error} + \operatorname{Bias}^2 + \operatorname{Variance}.$$

Irreducible Error

variance of the target around the true mean

Bias^2

Amount by which average

estimate differs from the true mean

Variance

Expected deviation of f^ around its mean

Bias-Variance Decomposition

Linear Model Fit: $\hat{f}_p(x) = \hat{\beta}^T x$

$$Err(x_0) = \sigma_{\varepsilon}^2 + \left[f(x_0) - E\hat{f}_p(x_0) \right]^2 + \left\| h(x_0) \right\|^2 \sigma_{\varepsilon}^2$$

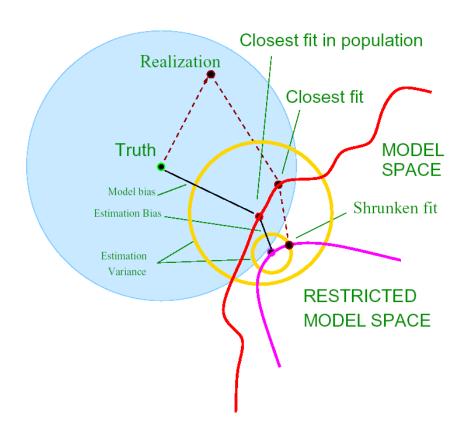
$$\mathbf{h}(x_0) = \mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} x_0$$

average over sample values x_i :

$$\frac{1}{N} \sum_{i=1}^{N} Err(x_i) = \sigma_{\varepsilon}^2 + \frac{1}{N} \sum_{i=1}^{N} \left[f(x_i) - E\hat{f}(x_i) \right]^2 + \frac{p}{N} \sigma_{\varepsilon}^2 \text{ ... in-sample error}$$

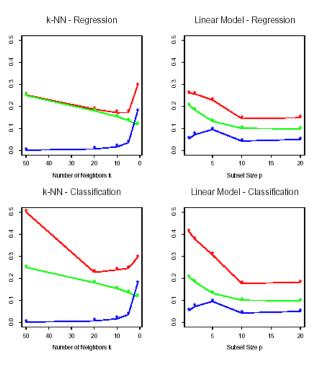
Model complexity is directly related to the number of parameters p

Bias-Variance Decomposition



Bias-Variance Decomposition - Example

ullet 50 observations. 20 predictors. Uniform in $egin{bmatrix} 0,1 \end{bmatrix}^{20}$



Left panels:

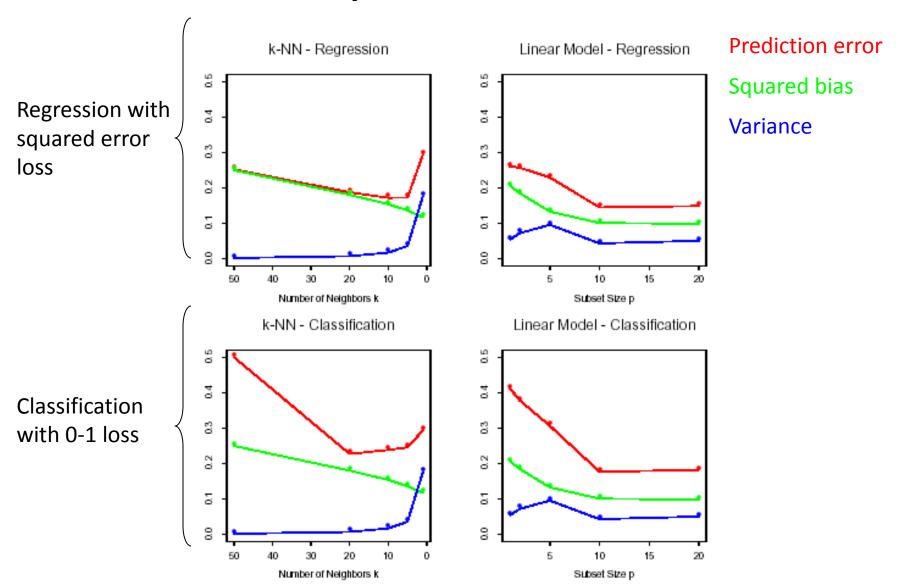
Y is 0 if $X_1 \le \frac{1}{2}$ and 1 if $X_1 > \frac{1}{2}$, and we apply kNN

Right panels

Y is 1 if $\sum_{j=1}^{10} X_j > 5$ and 0 otherwise, and we use the

best subset linear regression of size p

Example, continued



- Typically: training error rate < true error
- (same data is being used to fit the method and assess its error)

$$\overline{err} = \frac{1}{N} \sum_{i=1}^{n} L(y_i, \hat{f}(x_i)) < Err = E[L(Y, \hat{f}(X))]$$

overly optimistic

Err ... kind of <u>extra-sample</u> error: test features don't need to coincide with training feature vectors

Focus on in-sample error:

$$Err_{in} = \frac{1}{N} \sum_{i=1}^{N} E_{Y} E_{Y^{new}} L(Y_{i}^{new}, \hat{f}(x_{i}))$$

 $Y_{...}^{new}$ observe N **new** response values at each of training points

$$x_i$$
, i=1, 2, ...,N

optimism:
$$op \equiv Err_{in} - E_y(\overline{err})$$

for squared error 0-1 and other loss functions:

$$op = \frac{2}{N} \sum_{i=1}^{N} Cov(\hat{y}_i, y_i)$$

Summary:
$$Err_{in} = E_y(\overline{err}) + \frac{2}{N} \sum_{i=1}^{N} Cov(\hat{y}_i, y_i)$$

The harder we fit the data, the greater $Cov(\hat{y}_i, y_i)$ will be, thereby increasing the optimism.

For linear fit with d indep covariates:

$$Err_{in} = E_{y} \left(\overline{err} \right) + \frac{2}{N} d\sigma_{\varepsilon}^{2}$$

- optimism ♠ linearly with # d of covariates

- Ways to estimate prediction error:
 - Estimate optimism and then add it to training error rate
 - AIC, BIC, and others work this way, for a special class of estimates that are linear in their parameters
 - Direct estimates of the sample error
 - Cross-validation, bootstrap
 - Can be used with any loss function, and with nonlinear, adaptive fitting techniques

Estimates of In-Sample Prediction Error

General form of the in-sample estimate:

$$\hat{E}rr_{in} = \overline{err} + \hat{o}p$$

with estimate of optimism

• For linear fit and with $Err_{in} = E_y(\overline{err}) + \frac{2}{N}d\sigma_{\varepsilon}^2$:

$$C_p = \overline{err} + \frac{2d}{N} \hat{\sigma}_{\varepsilon}^2$$
, so called C_p statistic

 $\hat{\sigma}_{\varepsilon}^2$... estimate of noise variance, from mean-squared error of low-bias model

d... # of basis functions

N... training sample size

Estimates of In-Sample Prediction Error

- Similarly: Akaike Information Criterion (AIC)
 - More applicable estimate of Err_{in} , when log-likelihood function is used

For
$$N \to \infty$$
: $-2E \left[\log \Pr_{\hat{\theta}}(Y) \right] \approx -\frac{2}{N} E \left[\log \operatorname{lik} \right] + 2\frac{d}{N}$

 $Pr_{\theta}(Y)$... family density for Y (containing the true density)

 $\hat{\theta}$... ML estimate of θ

$$loglik = \sum_{i=1}^{N} log Pr_{\hat{\theta}}(y_i)$$
 Maximized log-likelihood due to ML estimate of theta

AIC

For
$$N \to \infty$$
: $-2E \left[\log \Pr_{\hat{\theta}}(Y) \right] \approx -\frac{2}{N} E \left[\log \operatorname{lik} \right] + 2\frac{d}{N}$

For example, for logistic regression model, using binomial log-likelihood:

$$AIC = -\frac{2}{N} \cdot \text{loglik} + 2 \cdot \frac{d}{N}$$

To use AIC for model selection: choose the model giving smallest AIC over the set of models considered.

$$AIC(\alpha) = \overline{err}(\alpha) + 2\frac{d(\alpha)}{N}\hat{\sigma}_{\varepsilon}^{2}$$

 $f_{\hat{\alpha}}(x)$... set of models, α ... tuning parameter $\overline{\text{err}}(\alpha)$... training error, $d(\alpha)$... # parameters

Effective Number of Parameters

$$y = \begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_N \end{pmatrix}$$
 Vector of Outcomes, similarly for predicitons

$$\hat{y} = Sy$$
 Linear fit (e.g. linear regression, quadratic shrinkage – ridge, splines)

 $S... N \times N$ matrix, depends on input vector x_i but not on y_i

effective number of parameters:
$$d(S) = trace(S)$$
 c.f. $Cov(\hat{y}, y)$

$$d(s)$$
 is the correct d for C_p

$$C_p = \overline{err} + \frac{2d}{N} \hat{\sigma}_{\varepsilon}^2$$

Bayesian Approach and BIC

Like AIC used in when fitting by max log-likelihood

Bayesian Information Criterion (BIC):

$$BIC = -2\log(1 + (\log N)d)$$

Assuming Gaussian model: σ_{ε}^2 known,

$$-2 \cdot \text{loglik} \approx \sum_{i} (y_{i} - \hat{f}(x_{i}))^{2} / \sigma_{\varepsilon}^{2} = N \cdot \overline{err} / \sigma_{\varepsilon}^{2}$$

then
$$BIC = \frac{N}{\sigma_{\varepsilon}^2} [\overline{err} + (\log N) \cdot \frac{d}{N} \sigma_{\varepsilon}^2]$$

BIC proportional to AIC except for log(N) rather than factor of 2. For $N>e^2$ (approx 7.4), BIC penalizes complex models more heavily.

BIC Motivation

- Given a set of candidate models $\mathbf{M}_m, m=1...M$ and model parameters θ_{m}
- Posterior probability of a given model: $Pr(\mathbf{M}_m \mid \mathbf{Z}) \propto Pr(\mathbf{M}_m) \cdot Pr(\mathbf{Z} \mid \mathbf{M}_m)$
- Where **Z** represents the training data $\{x_i, y_i\}_1^N$
- To compare two models, form the posterior odds:

$$\frac{\Pr(\mathbf{M}_{m} \mid \mathbf{Z})}{\Pr(\mathbf{M}_{l} \mid \mathbf{Z})} = \frac{\Pr(\mathbf{M}_{m})}{\Pr(\mathbf{M}_{l})} \cdot \frac{\Pr(\mathbf{Z} \mid \mathbf{M}_{m})}{\Pr(\mathbf{Z} \mid \mathbf{M}_{l})}$$

- If odds > 1, then choose model m. Prior over models (left half) considered constant. Right half, contribution of data (Z) to posterior odds, is called the Bayes factor BF(Z).
- Need to approximate $Pr(Z|M_m)$.
- Can est. posterior from BIC and compare relative merits of models.

General framework

$$Y_{i} = \sum_{j=1}^{p} \beta_{j}^{0} X_{i}^{(j)} + \varepsilon_{i}, i = 1, ..., n$$

$$p \gg n$$
in short: $\mathbf{Y} = \mathbf{X}\beta + \varepsilon$

goals:

- prediction, e.g. w.r.t. squared prediction error
- estimation of β^0 , e.g. w.r.t. $\|\hat{\beta} \beta^0\|_q$ (q = 1, 2)

Penalty based methods

if true β^0 is sparse w.r.t.

- ▶ $\|\beta^0\|_0^0$ = number of non-zero coefficients \sim regularize with the $\|\cdot\|_0$ -penalty: $\operatorname{argmin}_{\beta}(n^{-1}\|\mathbf{Y} - \mathbf{X}\beta\|^2 + \lambda \|\beta\|_0^0)$, e.g. AIC, BIC
 - \rightarrow computationally infeasible if p is large (2^p sub-models)
- ▶ $\|\beta^0\|_1 = \sum_{j=1}^p |\beta_j^0|$ \sim penalize with the $\|\cdot\|_1$ -norm, i.e. Lasso: $\operatorname{argmin}_{\beta}(n^{-1}\|\mathbf{Y} - \mathbf{X}\beta\|^2 + \lambda \|\beta\|_1)$
 - ~ convex optimization: computationally feasible and very fast for large p

The Lasso

Lasso for linear models

$$\hat{\beta}(\lambda) = \operatorname{argmin}_{\beta}(n^{-1} \|\mathbf{Y} - \mathbf{X}\beta\|^2 + \underbrace{\lambda}_{\geq 0} \underbrace{\|\beta\|_1}_{\sum_{j=1}^{\rho} |\beta_j|})$$

- → convex optimization problem
 - Lasso does variable selection some of the $\hat{\beta}_j(\lambda) = 0$ (because of " ℓ_1 -geometry")
 - $\hat{\beta}(\lambda)$ is a shrunken LS-estimate

The Lasso

equivalence to primal problem

$$\hat{\beta}_{\text{primal}}(R) = \operatorname{argmin}_{\beta; \|\beta\|_1 \le R} \|\mathbf{Y} - \mathbf{X}\beta\|_2^2 / n,$$

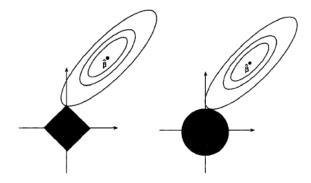
with a correspondence between λ and R which depends on the data $(X_1, Y_1), \ldots, (X_n, Y_n)$

since

- ▶ $\|\mathbf{Y} \mathbf{X}\beta\|_2^2/n$ is convex in β
- ▶ convex constraint $\|\beta\|_1 \le R$

The Lasso and the Ridge Regression





left: ℓ_1 -"world" residual sum of squares reaches a minimal value (for certain constellations of the data) if its contour lines hit the ℓ_1 -ball in its corner

$$\rightsquigarrow \hat{\beta}_1 = 0$$

The Lasso and the Ridge Regression

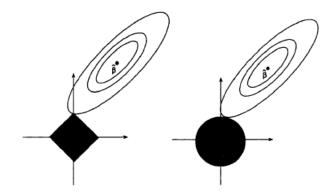
Ridge regression,

$$\hat{\beta}_{\text{Ridge}}(\lambda) = \operatorname{argmin}_{\beta} \left(\|\mathbf{Y} - \mathbf{X}\beta\|_{2}^{2} / n + \lambda \|\beta\|_{2}^{2} \right),$$

equivalent primal equivalent solution

$$\hat{\beta}_{\text{Ridge;primal}}(R) = \operatorname{argmin}_{\beta; \|\beta\|_2 \le R} \|\mathbf{Y} - \mathbf{X}\beta\|_2^2 / n,$$

with a one-to-one correspondence between λ and R



Relationship with Bayesian methods

model:

$$\beta_1, \ldots, \beta_p$$
 i.i.d. $\sim p(\beta)d\beta$, given β : $\mathbf{Y} \sim \mathcal{N}_n(\mathbf{X}\beta, \sigma^2 I_n)$ with density $f(\mathbf{y}|\sigma^2, \beta)$

posterior density:

$$p(\beta|\mathbf{Y},\sigma^2) = \frac{f(\mathbf{Y}|\beta,\sigma^2)p(\beta)}{\int f(\mathbf{Y}|\beta,\sigma^2)p(\beta)d\beta} \propto f(\mathbf{Y}|\beta,\sigma^2)p(\beta)$$

and hence for the MAP (Maximum A-Posteriori) estimator:

$$\hat{\beta}_{\text{MAP}} = \operatorname{argmax}_{\beta} p(\beta | \mathbf{Y}, \sigma^2) = \operatorname{argmin}_{\beta} - \log \left(f(\mathbf{Y} | \beta, \sigma^2) p(\beta) \right)$$

$$= \operatorname{argmin}_{\beta} \left(\frac{1}{2\sigma^2} ||\mathbf{Y} - X\beta||_2^2 - \sum_{j=1}^p \log(p(\beta_j)) \right)$$

Relationship with Bayesian methods

examples:

1. Double-Exponential prior $DExp(\xi)$:

$$p(\beta) = \frac{\tau}{2} \exp(-\tau \beta)$$

 $\rightarrow \hat{\beta}_{\text{MAP}}$ equals the Lasso with penalty parameter $\lambda = n^{-1}2\sigma^2\tau$

2. Gaussian prior $\mathcal{N}(0, \tau^2)$:

$$p(\beta) = \frac{1}{\sqrt{2\pi}\tau} \exp(-\beta^2/(2\tau^2))$$

 \rightarrow $\hat{\beta}_{\rm MAP}$ equals the Ridge estimator with penalty parameter $\lambda = n^{-1}\sigma^2/\tau^2$

but we will argue that Lasso (i.e., the MAP estimator) is also good if the truth is sparse with respect to $\|\beta^0\|_0^0$, e.g. if prior is (much) more spiky around zero than Double-Exponential distribution

Lasso for orthogonal design

$$\mathbf{Y} = \mathbf{X}\beta + \varepsilon, \quad n^{-1}\mathbf{X}^T\mathbf{X} = I$$

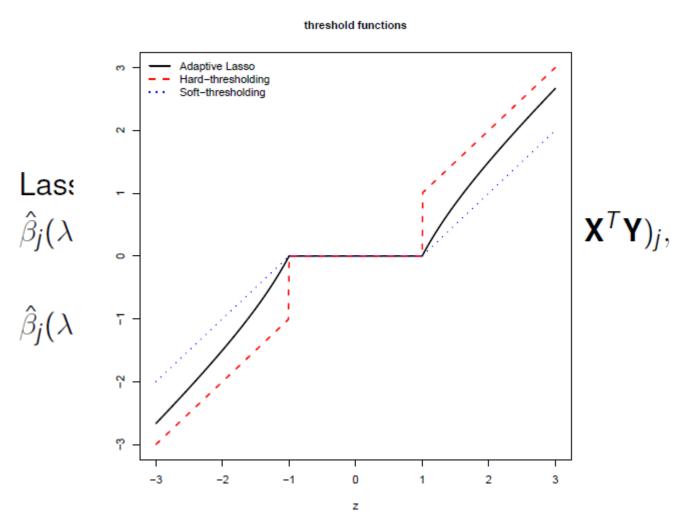
Lasso = soft-thresholding estimator

$$\hat{\beta}_j(\lambda) = \operatorname{sign}(Z_j)(|Z_j| - \lambda/2)_+, \ \underbrace{Z_j}_{=\operatorname{OLS}} = (n^{-1}\mathbf{X}^T\mathbf{Y})_j,$$

$$\hat{\beta}_j(\lambda) = g_{\text{soft}}(Z_j),$$

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Lasso for orthogonal design



Estimation of regression coefficients

$$\mathbf{Y} = \mathbf{X}\beta^0 + \varepsilon, \ p \gg n$$

with fixed (deterministic) design X

problem of identifiability:

for
$$p > n$$
: $\mathbf{X}\beta^0 = X\theta$ for any $\theta = \beta^0 + \xi$, ξ in the null-space of \mathbf{X}

 \sim cannot say anything about $\|\hat{\beta} - \beta^0\|$ without further assumptions!

→ we will work with the compatibility assumption (see later)
and we will explain: under compatibility condition

$$\|\hat{\beta} - \beta^0\|_1 \le C \frac{s_0}{\phi_0^2} \sqrt{\log(p)/n},$$

 $s_0 = |\sup(\beta^0)| = |\{j; \ \beta_i^0 \ne 0\}|$

Asymptotic Results-preview

for (fixed design) linear model $\mathbf{Y} = \mathbf{X}\beta^0 + \varepsilon$ with active set $S_0 = \{j; \ \beta_j^0 \neq 0\}$ two key assumptions

- neighborhood stability condition for design X
 ⇒ irrepresentable condition for design X
- 2. beta-min condition

$$\min_{j \in S_0} |\beta_j^0| \geq C\sqrt{s_0 \log(p)/n}$$
, C suitably large

both conditions are sufficient and "essentially" necessary for

$$\hat{S}(\lambda) = S_0$$
 with high probability, $\lambda \gg \sqrt{\log(p)/n}$

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Asymptotic Results

neighborhood stability condition ⇔ irrepresentable condition

$$n^{-1}\mathbf{X}^T\mathbf{X} = \hat{\Sigma}$$

active set $S_0 = \{j; \ \beta_j \neq 0\} = \{1, \dots, s_0\}$ consists of the first s_0 variables; partition

$$\hat{\Sigma} = \left(egin{array}{ccc} \hat{\Sigma}_{S_0,S_0} & \hat{\Sigma}_{S_0,S_0^c} \ \hat{\Sigma}_{S_0^c,S_0} & \hat{\Sigma}_{S_0^c,S_0^c} \end{array}
ight)$$

irrep. condition : $\|\hat{\Sigma}_{S_0^c,S_0}\hat{\Sigma}_{S_0,S_0}^{-1}\operatorname{sign}(\beta_1^0,\ldots,\beta_{s_0}^0)^T\|_{\infty} < 1$

Parameter Tuning

choice of λ : $\hat{\lambda}_{CV}$ from cross-validation empirical and theoretical indications (Meinshausen & PB, 2006) that

$$\hat{S}(\hat{\lambda}_{CV}) \supseteq S_0$$
 (or S_{relev})

moreover

$$|\hat{S}(\hat{\lambda}_{CV})| \leq \min(n, p) (= n \text{ if } p \gg n)$$

Parameter Tuning

recall:

$$\hat{S}(\hat{\lambda}_{CV}) \supseteq S_0$$
 (or S_{relev})

and we would then use a second-stage to reduce the number of false positive selections

 \sim re-estimation on much smaller model with variables from \hat{S}

- ▶ OLS on \hat{S} with e.g. BIC variable selection
- thresholding coefficients and OLS re-estimation
- adaptive Lasso (Zou, 2006)

...

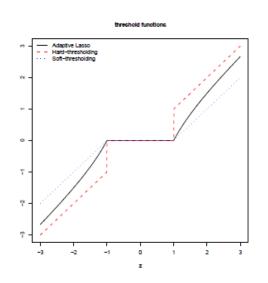
Adaptive Lasso

re-weighting the penalty function

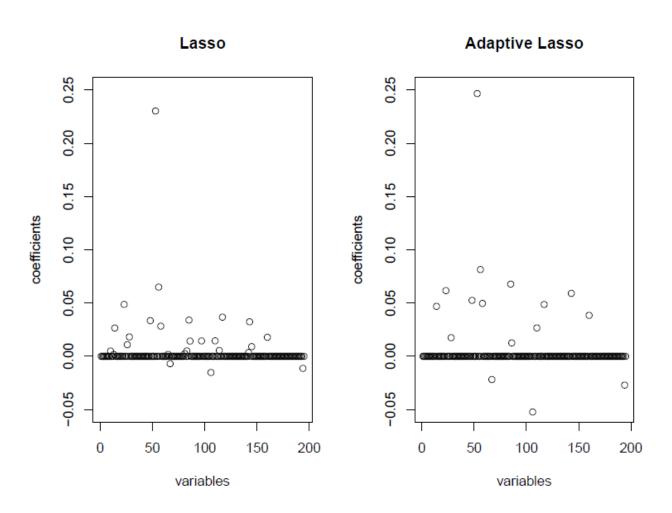
$$\hat{\beta} = \operatorname{argmin}_{\beta}(\|\mathbf{Y} - \mathbf{X}\beta\|_{2}^{2}/n + \lambda \sum_{j=1}^{p} \frac{|\beta_{j}|}{|\hat{\beta}_{init,j}|}),$$

$$\hat{\beta}_{init,j} \text{ from Lasso in first stage } \underbrace{(\text{or OLS if } p < n)}_{\text{Zou (2006)}}$$

for orthogonal design, if $\hat{\beta}_{init}$ = OLS: Adaptive Lasso = NN-garrote \rightarrow less bias than Lasso



Adaptive Lasso



KKT conditions and Computation

characterization of solution(s) $\hat{\beta}$ as minimizer of the criterion function

$$Q_{\lambda}(\beta) = \|\mathbf{Y} - \mathbf{X}\beta\|_{2}^{2}/n + \lambda \|\beta\|_{1}$$

since $Q_{\lambda}(\cdot)$ is a convex function: necessary and sufficient that subdifferential of $\partial Q_{\lambda}(\beta)/\partial \beta$ at $\hat{\beta}$ contains the zero element

Lemma

denote by $G(\beta) = -2\mathbf{X}^T(\mathbf{Y} - \mathbf{X}\beta)/n$ the gradient vector of $\|\mathbf{Y} - \mathbf{X}\beta\|_2^2/n$

Then: $\hat{\beta}$ is a solution if and only if

$$G_j(\hat{\beta}) = -\text{sign}(\hat{\beta}_j)\lambda \text{ if } \hat{\beta}_j \neq 0,$$

 $|G_j(\hat{\beta})| \leq \lambda \text{ if } \hat{\beta}_j = 0$

Coordinate descent algorithm for computation

general idea is to compute a solution $\hat{\beta}(\lambda_{\mathrm{grid},k})$ and use it as a starting value for the computation of $\hat{\beta}(\underbrace{\lambda_{\mathrm{grid},k-1}})$

 $\beta^{(0)} \in \mathbb{R}^p$ an initial parameter vector. Set m = 0.

REPEAT:

Increase m by one: $m \leftarrow m + 1$.

For j = 1, ..., p:

$$\begin{split} &\text{if } |G_j(\beta_{-j}^{(m-1)})| \leq \lambda: \text{ set } \beta_j^{(m)} = 0, \\ &\text{otherwise: } \beta_j^{(m)} = \operatorname{argmin}_{\beta_j} Q_\lambda(\beta_{+j}^{(m-1)}), \end{split}$$

 β_{-j} : parameter vector setting jth component to zero $\beta_{+j}^{(m-1)}$: parameter vector which equals $\beta^{(m-1)}$ except for jth component equalling β_j UNTIL numerical convergence

Coordinate descent algorithm for computation

For linear regression

$$G_{j}(\beta) = -2\mathbf{X}_{j}^{T}(\mathbf{Y} - \mathbf{X}\beta)/n$$

$$\beta_{j}^{(m)} = \frac{\operatorname{sign}(Z_{j})(|Z_{j}| - \lambda/2)_{+}}{\hat{\Sigma}_{jj}},$$

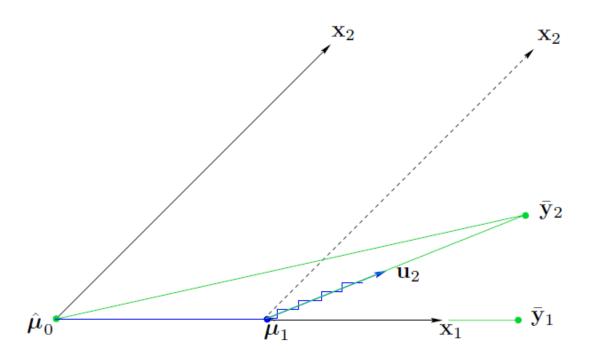
$$Z_{j} = \mathbf{X}_{j}^{T}(\mathbf{Y} - \mathbf{X}\beta_{-j})/n, \quad \hat{\Sigma} = n^{-1}\mathbf{X}^{T}\mathbf{X}.$$

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→ componentwise soft-thresholding

glmnet: R-package

- 1. Start with $r = y, \hat{\beta}_1, \hat{\beta}_2, \dots \hat{\beta}_p = 0$. Assume x_j standardized.
- 2. Find predictor x_i most correlated with r.
- 3. Increase β_j in the direction of $\operatorname{sign}\langle r, x_j \rangle$ until some other competitor x_k has as much correlation with current residual as does x_j .
- 4. Move $(\hat{\beta}_j, \hat{\beta}_k)$ in the joint least squares direction for (x_j, x_k) until some other competitor x_ℓ has as much correlation with the current residual
- 5. Continue in this way until all predictors have been entered. Stop when $\langle r, x_j \rangle = 0 \,\forall j$, i.e. OLS solution.



The LAR direction \mathbf{u}_2 at step 2 makes an equal angle with \mathbf{x}_1 and \mathbf{x}_2 .

For each iteration, we have:

- Active set A_k at the beginning of the kth step
- Coefficient vector β_{A_k} at this step
- k-1 nonzero values, the one just entered the model has coefficient 0.

Then we do:

- Compute current residual $\mathbf{r}_k = \mathbf{y} \mathbf{X}_{\mathcal{A}_k} \beta_{\mathcal{A}_k}$;
- Compute direction $\delta_k = (\mathbf{X}_{\mathcal{A}_k}^T \mathbf{X}_{\mathcal{A}_k})^{-1} \mathbf{X}_{\mathcal{A}_k}^T \mathbf{r}_k$;
- Evolve the coefficient $\beta_{\mathcal{A}_k}(\alpha) = \beta_{\mathcal{A}_k} + \alpha \cdot \delta_k$ until some \mathbf{x}_l has as much correlation with the current residual.
- Add \mathbf{x}_l to the active set \mathcal{A}_{k+1}

Algorithm 3.2a Least Angle Regression: Lasso Modification.

4a. If a non-zero coefficient hits zero, drop its variable from the active set of variables and recompute the current joint least squares direction.

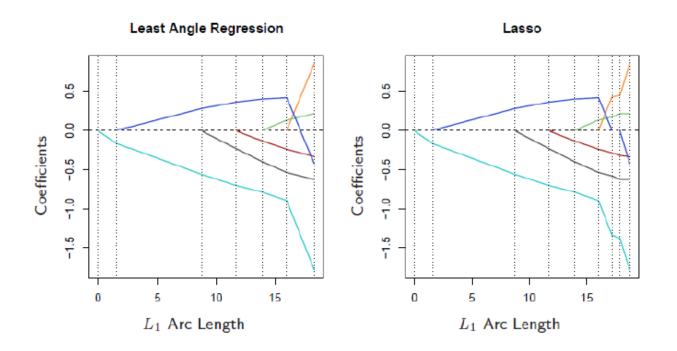


FIGURE 3.15. Left panel shows the LAR coefficient profiles on the simulated data, as a function of the L_1 arc length. The right panel shows the Lasso profile. They are identical until the dark-blue coefficient crosses zero at an arc length of about 18.

Generalization of Lasso and Ridge regression

Consider:

$$\tilde{\beta} = \operatorname{Argmin}_{\beta} \left\{ \sum_{i=1}^{N} (y_i - \beta_0 - \sum_{j=1}^{p} x_{ij} \beta_j)^2 + \lambda \sum_{j=1}^{p} |\beta_j|^q \right\}$$

- $|\beta_j|^q$ prior distribution for β_j ,
- $\mathbf{q} = 1$ smallest q that constraint is still convex,
- Typically q = 1, 2 (Lasso and Ridge regression).
- **a** can be determined by data, but not worth the effort.

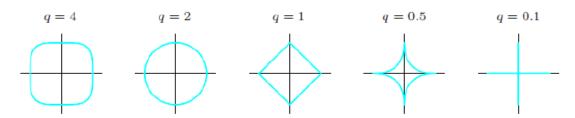


FIGURE 3.12. Contours of constant value of $\sum_{j} |\beta_{j}|^{q}$ for given values of q.

The Dantzig Selector

Candes and Tao (2007) proposed the Dantzig Selector (DS):

$$\min_{\beta} \|\beta\|_1 \text{ subject to } \|\mathbf{X}^T(\mathbf{y} - \mathbf{X}\beta)\|_{\infty} \leq s$$

It can also be written as:

$$\min_{\beta} \|\mathbf{X}^T(\mathbf{y} - \mathbf{X}\beta)\|_{\infty}$$
 subject to $\|\beta\|_1 \le t$

The grouped Lasso

Suppose the p predictors are divided into L groups, with p_{ℓ} the number in group ℓ . The grouped-Lasso solves the minimization problem:

$$\min_{\beta \in \mathbb{R}^p} \left(\|\mathbf{y} - \beta_0 \mathbf{1} - \sum_{\ell=1}^L \mathbf{X}_\ell \beta_\ell \|_2^2 + \lambda \sum_{\ell=1}^L \sqrt{p_\ell} \|\beta_\ell\|_2 \right)$$

where X_{ℓ} is the predictors corresponding to the ℓ th group, with corresponding coefficient vector β_{ℓ} .

In Linear regression:

The true sparse model

$$\mathcal{M}_* = \{ 1 \leqslant i \leqslant p : \beta_i \neq 0 \}$$
$$\omega = \mathbf{X}^{\mathsf{T}} \mathbf{y}$$

 $\mathcal{M}_{\gamma} = \{1 \leq i \leq p : |\omega_i| \text{ is among the first } [\gamma n] \text{ largest of all} \}$ $\gamma \in (0, 1)$

Need to show

$$P(\mathcal{M}_* \subset \mathcal{M}_\gamma) \to 1$$
 as $n \to \infty$

Rationale of correlation learning:

When p > n, the OLS estimator

$$\hat{\beta}_{LS} = (\mathbf{X}^T \mathbf{X})^{+} \mathbf{X}^T \mathbf{y}$$
 is noisy

(X^TX)⁺ is the Moore-Penrose generalized inverse

The ridge regression

$$\omega^{\lambda} = (\mathbf{X}^{\mathsf{T}} \mathbf{X} + \lambda I_p)^{-1} \mathbf{X}^{\mathsf{T}} \mathbf{y}$$

$$\omega^{\lambda} \to \hat{\beta}_{\mathsf{LS}} \qquad \text{as } \lambda \to 0,$$

$$\lambda \omega^{\lambda} \to \omega \qquad \text{as } \lambda \to \infty.$$

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Iteratively thresholded ridge regression screener (ITRRS)

$$\mathcal{M}_{\delta,\lambda}^{1} = \{1 \leq i \leq p : |\omega_{i}^{\lambda}| \text{ is among the first } [\delta p] \text{ largest of all}\}.$$
 (8)

- (a) First, carry out the procedure in submodel (8) to the full model $\{1, \ldots, p\}$ and obtain a submodel $\mathcal{M}_{\delta,\lambda}^1$ with size $[\delta p]$.
- (b) Then, apply a similar procedure to the model $\mathcal{M}^1_{\delta,\lambda}$ and again obtain a submodel $\mathcal{M}^2_{\delta,\lambda} \subset \mathcal{M}^1_{\delta,\lambda}$ with size $[\delta^2 p]$, and so on.
- (c) Finally, obtain a submodel $\mathcal{M}_{\delta,\lambda} = \mathcal{M}_{\delta,\lambda}^k$ with size $d = [\delta^k p] < n$, where $[\delta^{k-1} p] \ge n$.

Theorem 1 (accuracy of SIS). Under conditions 1–4, if $2\kappa + \tau < 1$ then there is some $\theta < 1 - 2\kappa - \tau$ such that, when $\gamma \sim cn^{-\theta}$ with c > 0, we have, for some C > 0,

$$P(\mathcal{M}_* \subset \mathcal{M}_\gamma) = 1 - O[\exp\{-Cn^{1-2\kappa}/\log(n)\}].$$

Theorem 2 (asymptotic sure screening). Under conditions 1–4, if $2\kappa + \tau < 1$, $\lambda(p^{3/2}n)^{-1} \to \infty$, and $\delta n^{1-2\kappa-\tau} \to \infty$ as $n \to \infty$, then we have, for some C > 0,

$$P(\mathcal{M}_* \subset \mathcal{M}^1_{\delta,\lambda}) = 1 - O[\exp\{-Cn^{1-2\kappa}/\log(n)\}].$$

Condition 1. p > n and $\log(p) = O(n^{\xi})$ for some $\xi \in (0, 1 - 2\kappa)$, where κ is given by condition 3.

Condition 2. **z** has a spherically symmetric distribution and property C. Also, $\varepsilon \sim \mathcal{N}(0, \sigma^2)$ for some $\sigma > 0$.

Condition 3. var(Y) = O(1) and, for some $\kappa \ge 0$ and $c_2, c_3 > 0$,

$$\min_{i \in \mathcal{M}_*} |\beta_i| \geqslant \frac{c_2}{n^{\kappa}} \quad \text{and} \quad \min_{i \in \mathcal{M}_*} |\operatorname{cov}(\beta_i^{-1} Y, X_i)| \geqslant c_3.$$

As seen later, κ controls the rate of probability error in recovering the true sparse model. Although $b = \min_{i \in \mathcal{M}_*} |\text{cov}(\beta_i^{-1}Y, X_i)|$ is assumed here to be bounded away from 0, our asymptotic study applies as well to the case where $b \to 0$ as $n \to \infty$. In particular, when the variables in \mathcal{M}_* are uncorrelated, b = 1. This condition rules out the situation in which an important variable is marginally uncorrelated with Y, but jointly correlated with Y.

Condition 4. There are some $\tau \ge 0$ and $c_4 > 0$ such that

$$\lambda_{\max}(\Sigma) \leqslant c_4 n^{\tau}$$
.

$$\Sigma = \text{cov}(\mathbf{x})$$

S=8, 18

p			Results for the fo	llowing method	ls:	
	Dantzig selector	Lasso	SIS–SCAD	SIS–DS	SIS–DS– SCAD	SIS–DS– AdaLasso
1000 20000	10 ³ (1.381)	62.5 (0.895) —	15 (0.374) 37 (0.288)	37 (0.795) 119 (0.732)	27 (0.614) 60.5 (0.372)	34 (1.269) 99 (1.014)

Szekely, Rizzo and Bakirov (2007) proposed the distance correlation

$$\operatorname{dcov}^{2}(\mathbf{u}, \mathbf{v}) = \int_{R^{d_{u}+d_{v}}} \|\phi_{\mathbf{u}, \mathbf{v}}(\mathbf{t}, \mathbf{s}) - \phi_{\mathbf{u}}(\mathbf{t})\phi_{\mathbf{v}}(\mathbf{s})\|^{2} w(\mathbf{t}, \mathbf{s}) d\mathbf{t} d\mathbf{s},$$

$$\phi_{\mathbf{u}}(\mathbf{t}) \ \phi_{\mathbf{v}}(\mathbf{s}) \ \phi_{\mathbf{u},\mathbf{v}}(\mathbf{t},\mathbf{s})$$

characteristic functions of two random vectors

$$w(\mathbf{t}, \mathbf{s}) = \left\{ c_{d_u} c_{d_v} \|\mathbf{t}\|_{d_u}^{1+d_u} \|\mathbf{s}\|_{d_v}^{1+d_v} \right\}^{-1}$$

$$dcorr(\mathbf{u}, \mathbf{v}) = \frac{dcov(\mathbf{u}, \mathbf{v})}{\sqrt{dcov(\mathbf{u}, \mathbf{u})dcov(\mathbf{v}, \mathbf{v})}}$$

For two normal random variables

$$= \left\{ \frac{\rho \arcsin(\rho) + \sqrt{1 - \rho^2} - \rho \arcsin(\rho/2) - \sqrt{4 - \rho^2} + 1}{1 + \pi/3 - \sqrt{3}} \right\}^{1/2}$$

Distance correlation is strictly increasing in $|\rho|$

$$dcov^{2}(\mathbf{u}, \mathbf{v}) = S_{1} + S_{2} - 2S_{3},$$

$$S_{1} = E\{\|\mathbf{u} - \widetilde{\mathbf{u}}\|_{d_{u}}\|\mathbf{v} - \widetilde{\mathbf{v}}\|_{d_{v}}\},$$

$$S_{2} = E\{\|\mathbf{u} - \widetilde{\mathbf{u}}\|_{d_{u}}\}E\{\|\mathbf{v} - \widetilde{\mathbf{v}}\|_{d_{v}}\}, \text{ and }$$

$$S_{3} = E\{E(\|\mathbf{u} - \widetilde{\mathbf{u}}\|_{d_{u}}\|\mathbf{u})E(\|\mathbf{v} - \widetilde{\mathbf{v}}\|_{d_{v}}\|\mathbf{v})\},$$

$$(\widetilde{\mathbf{u}}, \widetilde{\mathbf{v}}) \text{ is an independent copy of } (\mathbf{u}, \mathbf{v}).$$

$$\widehat{S}_{1} = \frac{1}{n^{2}} \sum_{i=1}^{n} \sum_{j=1}^{n} \|\mathbf{u}_{i} - \mathbf{u}_{j}\|_{d_{u}} \|\mathbf{v}_{i} - \mathbf{v}_{j}\|_{d_{v}},$$

$$\widehat{S}_{2} = \frac{1}{n^{2}} \sum_{i=1}^{n} \sum_{j=1}^{n} \|\mathbf{u}_{i} - \mathbf{u}_{j}\|_{d_{u}} \frac{1}{n^{2}} \sum_{i=1}^{n} \sum_{j=1}^{n} \|\mathbf{v}_{i} - \mathbf{v}_{j}\|_{d_{v}},$$

$$\widehat{S}_{3} = \frac{1}{n^{3}} \sum_{i=1}^{n} \sum_{j=1}^{n} \sum_{i=1}^{n} \sum_{l=1}^{n} \|\mathbf{u}_{i} - \mathbf{u}_{l}\|_{d_{u}} \|\mathbf{v}_{j} - \mathbf{v}_{l}\|_{d_{v}}.$$

$$\widehat{\operatorname{dcov}}^{2}(\mathbf{u}, \mathbf{v}) = \widehat{S}_{1} + \widehat{S}_{2} - 2\widehat{S}_{3}.$$

$$\widehat{\operatorname{dcorr}}(\mathbf{u}, \mathbf{v}) = \frac{\widehat{\operatorname{dcov}}(\mathbf{u}, \mathbf{v})}{\sqrt{\operatorname{dcov}(\mathbf{u}, \mathbf{u})\operatorname{dcov}(\mathbf{v}, \mathbf{v})}}.$$

$$\mathcal{D} = \{k : F(\mathbf{y} \mid \mathbf{x}) \text{ functionally depends on } X_k \text{ for some } \mathbf{y} \in \Psi_y\},$$

$$\mathcal{I} = \{k : F(\mathbf{y} \mid \mathbf{x}) \text{ does not functionally depend on } X_k \text{ for any } \mathbf{y} \in \Psi_y\}.$$
 (2.5)

$$\omega_k = \operatorname{dcorr}^2(X_k, \mathbf{y}), \quad \text{and} \quad \widehat{\omega}_k = \widehat{\operatorname{dcorr}}^2(X_k, \mathbf{y}).$$

$$\widehat{\mathcal{D}}^{\star} = \{k : \widehat{\omega}_k \ge cn^{-\kappa}, \text{ for } 1 \le k \le p\}$$

Li et al. (2012) JASA

Theorem 1. Under Condition (C1), for any $0 < \gamma < 1/2 - \kappa$, there exist positive constants $c_1 > 0$ and $c_2 > 0$ such that

$$\Pr\left(\max_{1 \le k \le p} \left| \widehat{\omega}_k - \omega_k \right| \ge cn^{-\kappa} \right)$$

$$\le O(p[\exp\{-c_1 n^{1 - 2(\kappa + \gamma)}\} + n \exp(-c_2 n^{\gamma})]). \quad (2.6)$$

Under Conditions (C1) and (C2), we have that

$$\Pr\left(\mathcal{D}\subseteq\widehat{\mathcal{D}}^{\star}\right)\geq 1-O(s_n[\exp\{-c_1n^{1-2(\kappa+\gamma)}\}+n\exp(-c_2n^{\gamma})]),$$

(C1) Both **x** and **y** satisfy the subexponential tail probability uniformly in p. That is, there exists a positive constant s_0 such that for all $0 < s \le 2s_0$,

$$\sup_{p} \max_{1 \le k \le p} E\left\{ \exp\left(s \|X_k\|_1^2\right) \right\} < \infty, \quad \text{and}$$

$$E\left\{ \exp\left(s \|\mathbf{y}\|_q^2\right) \right\} < \infty.$$

(C2) The minimum DC of active predictors satisfies

$$\min_{k\in\mathcal{D}}\omega_k\geq 2cn^{-\kappa},$$

for some constants c > 0 and $0 \le \kappa < 1/2$.

(1.a):
$$Y = c_1\beta_1X_1 + c_2\beta_2X_2 + c_3\beta_3\mathbf{1}(X_{12} < 0) + c_4\beta_4X_{22} + \varepsilon,$$

(1.b): $Y = c_1\beta_1X_1X_2 + c_3\beta_2\mathbf{1}(X_{12} < 0) + c_4\beta_3X_{22} + \varepsilon,$
(1.c): $Y = c_1\beta_1X_1X_2 + c_3\beta_2\mathbf{1}(X_{12} < 0)X_{22} + \varepsilon,$
(1.d): $Y = c_1\beta_1X_1 + c_2\beta_2X_2 + c_3\beta_3\mathbf{1}(X_{12} < 0) + \exp(c_4|X_{22}|)\varepsilon,$

Table 1. The 5%, 25%, 50%, 75%, and 95% quantiles of the minimum model size S out of 500 replications in Example 1

\mathcal{S}	SIS					SIRS				DC-SIS					
Model	5%	25%	50%	75%	95%	5%	25%	50%	75%	95%	5%	25%	50%	75%	95%
					C	ase 1: <i>p</i>	= 2000 a	and $\sigma_{ij} =$	$0.5^{ i-j }$						
(1.a)	4.0	4.0	5.0	7.0	21.2	4.0	4.0	5.0	7.0	45.1	4.0	4.0	4.0	6.0	18.0
(1.b)	68.0	578.5	1180.5	1634.5	1938.0	232.9	871.5	1386.0	1725.2	1942.4	5.0	9.0	24.5	73.0	345.1
(1.c)	395.9	1037.2	1438.0	1745.0	1945.1	238.5	805.0	1320.0	1697.0	1946.0	6.0	10.0	22.0	59.0	324.1
(1.d)	130.5	611.2	1166.0	1637.0	1936.5	42.0	304.2	797.0	1432.2	1846.1	4.0	5.0	9.0	41.0	336.2
					C	ase 2: <i>p</i>	= 2000	and $\sigma_{ij} =$	$0.8^{ i-j }$						
(1.a)	5.0	9.0	16.0	97.0	729.4	5.0	9.0	18.0	112.8	957.1	4.0	7.0	11.0	31.2	507.2
(1.b)	26.0	283.2	852.0	1541.2	1919.0	103.9	603.0	1174.0	1699.2	1968.0	5.0	8.0	11.0	17.0	98.0
(1.c)	224.5	775.2	1249.5	1670.0	1951.1	118.6	573.2	1201.5	1685.2	1955.0	7.0	10.0	15.0	38.0	198.3
(1.d)	79.0	583.8	1107.5	1626.2	1930.0	50.9	300.5	728.0	1368.2	1900.1	4.0	7.0	17.0	73.2	653.1
					C	ase 3: <i>p</i>	= 5000	and $\sigma_{ij} =$	$0.5^{ i-j }$						
(1.a)	4.0	4.0	5.0	6.0	59.0	4.0	4.0	5.0	7.0	88.4	4.0	4.0	4.0	6.0	34.1
(1.b)	165.1	1112.5	2729.0	3997.2	4851.5	560.8	1913.0	3249.0	4329.0	4869.1	5.0	11.8	45.0	168.8	956.7
(1.c)	1183.7	2712.0	3604.5	4380.2	4885.0	440.4	1949.0	3205.5	4242.8	4883.1	7.0	17.0	53.0	179.5	732.0
(1.d)	259.9	1338.5	2808.5	3990.8	4764.9	118.7	823.2	1833.5	3314.5	4706.1	4.0	5.0	15.0	77.2	848.2
					C	ase 4: <i>p</i>	= 5000	and $\sigma_{ii} =$	$0.8^{ i-j }$						
(1.a)	5.0	10.0	26.5	251.5	2522.7	5.0	10.0	28.0	324.8	3246.4	5.0	8.0	14.0	69.0	1455.1
(1.b)	40.7	639.8	2072.0	3803.8	4801.7	215.7	1677.8	3010.0	4352.2	4934.1	5.0	8.0	11.0	21.0	162.0
(1.c)	479.2	1884.8	3347.5	4298.5	4875.2	297.7	1359.2	2738.5	4072.5	4877.6	8.0	12.0	22.0	83.0	657.9
(1.d)	307.0	1544.0	2832.5	4026.2	4785.2	148.2	672.0	1874.0	3330.0	4665.2	4.0	7.0	21.0	165.2	1330.0

Bayesian Methods

See Blackboard