Perspectives on Machine Bias Versus Human Bias: Generalized Linear Models

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Current Challenges in Statistical Learning BIRS

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Executive Summary

Proposed Estimation Strategies

Model Selection and Post Estimation

Simulation Study

Application: South African Heart Disease Data

Envo

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- Consider a set of observations $\mathbf{Y} = (y_1, y_2, \dots, y_n)'$, where y_i is assumed to have a distribution in the exponential family of distributions with predictor values $\mathbf{x}_i = (x_{i1}, x_{i2}, \dots, x_{in})'$.
- The probability density/mass function of the form

$$f_Y(y_i; \theta_i, \phi) = \exp\{(y_i\theta_i - b(\theta_i))/a_i(\phi) + c(y_i, \phi)\}$$

where $a(\cdot)$, $b(\cdot)$ and $c(\cdot)$ are known functions and ϕ is a scale parameter. If ϕ is known, then the exponential-family model with canonical parameter θ_i can be written as

$$f_Y(y_i; \theta_i) = c(y_i) exp\{y_i\theta_i - b(\theta_i)\}$$

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Some key features for Generalized Linear Model(GLIM)

- The random component of a GLIM specifies the distribution of the response variable Y_i
- The mean and variance of the response variable Y_i are given by

$$E[Y_i] = \mu_i = \frac{db(\theta_i)}{d\theta_i}$$
 and $Var(Y_i) = V(\mu_i) = \frac{d^2b(\theta_i)}{d\theta_i^2}$.

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The link function connects the random and systematic components. This connection is done by equating the mean response μ_i to the linear predictor η_i by $\eta_i = g(\mu_i)$, that is

$$g(\mu_i) \stackrel{\textit{link}}{=} \eta_i = \mathbf{x}_i' \boldsymbol{\beta}.$$

Candidate Subspace

A Great Deal of Redundancy in the Full Model

We want to estimate eta when it is plausible that eta lie in the subspace

$$H\beta = h$$

Hence the Non-Sample information (NSI) or Uncertain prior information (UPI)is

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H is $q \times k$ matrix of rank $q \leq k$

h is a given $q \times 1$ vector of constants.

Genomics Research

The goal of this paper is to analyze some of the issues involved in the estimation of the parameters in generalized linear models that may be over-parameterized that is, too many \mathbf{x} 's and thus $\boldsymbol{\beta}$'s are included.

For example, in genomics research it is common practice to test a candidate subset of genetic markers for association with disease. Here the candidate subset is found in a certain population by doing genome wide association studies. The candidate subset is then tested for disease association in a new population. In this new population it is possible that genetic markers not found in the first population are associated with disease.

Coronary Heart Disease (CHD) Data

Consider a data set which is analyzed by Park and Hastie (2006) [this data set is originally collected by Rossouw (1983)].

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- Low density
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Two key aspects of variable selection methods are:

- Evaluating each potential subset of predictor variables
- Deciding on the collection of potential subsets

- R²- Adjusted
- Akaike's Information Criterion (AIC)
- Corrected AIC
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- The log-likelihood is given by

$$I(\beta) = \sum_{i=1}^{n} \left[\left(y_i \theta_i - b(\theta_i) \right) + \log c(y_i) \right]$$

• The score equations are given by

$$(\mathbf{Y} - \boldsymbol{\mu})' \mathbf{D}(\boldsymbol{\mu}) \mathbf{X} = \mathbf{0},$$

where
$$\mathbf{D}(\mu) = \operatorname{diag}(d_{ii})$$
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The Candidate Estimator

- The score equations cannot be solved explicitly and hence recourse must be made numerical methods to get unrestricted maximum likelihood estimate (UE), $\hat{\beta}$.
- There are at least three methods available to solve these equations:
- The Newton-Raphson method
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- To get this estimator we need to maximize the log-likelihood under the restrictions $\mathbf{H}\beta = \mathbf{h}$.
- Using penalty function method to form a modified likelihood:

$$F(\beta, \lambda) = \sum_{i=1}^{n} \left[(y_i \theta_i - b(\theta_i)) + \log c(y_i) \right] + \sum_{j=1}^{q} \rho_j (\mathbf{h}_j - \mathbf{H}'_j \beta)^2.$$

- Find the solution of $\max_{\beta} F(\beta, \lambda)$ for positive and fixed values of p_i , $j = 1, \dots, q$.
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The restricted estimator $\tilde{\boldsymbol{\beta}}$ is

$$\tilde{\boldsymbol{\beta}} = \hat{\boldsymbol{\beta}} + (\mathbf{X}'\mathbf{W}\mathbf{X})^{-1}\mathbf{H}' \left[\mathbf{H}(\mathbf{X}'\mathbf{W}\mathbf{X})^{-1}\mathbf{H}'\right]^{-1} [\mathbf{h} - \mathbf{H}\hat{\boldsymbol{\beta}}].$$

Under some regularity conditions, it may be showed that that $\tilde{\beta}$ is a consistent estimator of β , and

$$\begin{split} \sqrt{n}(\tilde{\boldsymbol{\beta}} - \boldsymbol{\beta}) & \stackrel{d}{\longrightarrow} N_k \left(\boldsymbol{0}, \tilde{\boldsymbol{J}}^{-1} \right), \\ \tilde{\boldsymbol{J}}^{-1} &= (\boldsymbol{X}'\boldsymbol{W}\boldsymbol{X})^{-1} \left[\boldsymbol{I} - \boldsymbol{H}' \{ \boldsymbol{H} (\boldsymbol{X}'\boldsymbol{W}\boldsymbol{X})^{-1} \boldsymbol{H}' \}^{-1} \boldsymbol{H} (\boldsymbol{X}'\boldsymbol{W}\boldsymbol{X})^{-1} \right] \end{split}$$

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Pooling Data: Making Sense or Folly?

- Can ginseng prevent colds?
- Edmonton company CV Technologies Inc. has conducted clinical trials, with results published in the Journal of the American Geriatrics Society showing that their proprietary ginseng extract can prevent colds.
- Later, an article was published in the Vancouver Sun, in which two researchers from the UBC criticized the claims.
- They suggested that trials do not provide definite evidence that the product had any effect.

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Torturing Data Until it Confesses

- The study consisted of two randomized clinical trials (2000 and 2001), with nursing-home patients as subjects.
- In each trial, the subjects were randomly assigned to take either 200 mg of the ginseng extract or a placebo twice daily.
- The trials were conducted as double-blind studies.
- It obtained results that indicated a reduction in laboratory-confirmed respiratory illness (colds and flu).
- Results were statistically significant.

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- Combining the two studies erodes the credibility of the results: Taking two studies that do not show a benefit and then adding them together to get a positive result is a form of data-mining. It's torturing the data until it confesses.
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Hypothesis Testing

$$H_0: \mathbf{H}\boldsymbol{\beta} = \mathbf{h} \qquad H_a: \mathbf{H}\boldsymbol{\beta} \neq \mathbf{h}$$

Test Statistics

Likelihood Ratio Test (LRT)

$$D = 2[l(\hat{\beta}; y_1, \dots, y_n) - l(\tilde{\beta}; y_1, \dots, y_n)]$$

= $(\mathbf{H}\hat{\beta} - \mathbf{h})'\mathbf{H}(\mathbf{X}'\mathbf{W}\mathbf{X})^{-1}\mathbf{H}'(\mathbf{H}\hat{\beta} - \mathbf{h}) + o_p(1)$

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- Variable selection via penalized estimation is appealing for dimension reduction.
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LASSO

• It is a constrained version of ordinary least squares. The LASSO estimate $\hat{\beta}(\lambda)$ is the solution to

$$\hat{\boldsymbol{\beta}}_{\lambda} = \min_{\boldsymbol{\beta}} (\mathbf{y} - \mathbf{x}'\boldsymbol{\beta})'(\mathbf{y} - \mathbf{x}'\boldsymbol{\beta}) \quad \text{subject to} \quad \sum_{j=1}^{p} |\beta_j| \leq s,$$

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An alternative formulation of the LASSO is to solve the penalized likelihood problem

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- Alternatively, for small values of s (or equivalently large values of λ) some of these resulting estimated regressions coefficient are exactly zero, effectively (?) omitting predictor variables from the model.
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- They showed that under appropriate conditions, the LASSO estimators are consistent for estimating the regression coefficients, and the limit distribution of the LASSO estimators can have positive probability mass at 0 when the true value of the parameter is 0.

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- It is a useful tool for selecting variables according to the amount of penalization on the L₁ norm of the coefficients
- It is similar to the LASSO strategy

$$\hat{\beta}(\lambda) = \underset{\beta}{\operatorname{argmin}} \{-l(\beta) + \lambda ||\beta||_{1}\}$$

$$= -\sum_{i=1}^{n} [(y_{i}\theta_{i} - b(\theta_{i})) + \log c(y_{i})] + \lambda ||\beta||_{1},$$

- $\lambda > 0$ is the regularization parameter.
- If $\lambda = 0$, this just gives the maximum likelihood estimates.
- However, larger values of λ produce shrunken estimate of β , often with many components equal to zero.

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The maximum likelihood solution for the natural parameter θ , and thus β , with a penalization on the size of the L_1 norm of the coefficients $(||\beta||_1)$ i.e.,

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The adaptive L_1 GLM is the solution of

$$\hat{\boldsymbol{\beta}}_{\lambda}^{AL_{1}} = -\sum_{i=1}^{n} \left[(y_{i}\theta_{i} - b(\theta_{i})) + \ln c(y_{i}) \right] + \lambda \sum_{i=1}^{k} |\beta_{i}| w_{i},$$

where w_i 's are adaptive weights defined as $w_i = |\hat{\beta}_i|^{-\tau}$ for some positive τ , and $\hat{\beta}_i$ is the maximizer of the log likelihood.

- The intuition idea of the adaptive L₁GLM is that, by allowing a relatively higher penalty for coefficients inactive predictors and lower penalty for coefficients of active predictors, it is possible to reduce the estimation bias and improve variable selection accuracy, compared with the standard LASSO.
- Theoretically, adaptive L₁GLM enjoys oracle properties (Zou, 2006) that LASSO does not have.
- When k is fixed and $n \to \infty$, with some selected λ , then the adaptive L_1 GLM selects the true model with probability tending to one.

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- ullet This method selects variables and estimate parameters eta simultaneously by maximizing the penalized likelihood function

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$$p_{\lambda}'(\theta) = \lambda \left[I(\theta \le \lambda) + \frac{(a\lambda - \theta)_{+}}{(a - 1)\lambda} I(\theta > \lambda) \right].$$

where a is some constant usually taken to be a=3.7 and $(t)_+=t/\{t>0\}$ is the hinge loss function.

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- Regardless of sample size, the model selection step typically has a dramatic effect on the sampling properties of the estimators.
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- Despite some claims to contrary, no model selection procedure either implemented on a machine or not is immune to these difficulties.[Leeb and Potscher, 2005]

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Asymptotic Treatment

Consider a sequence $K_{(n)}$ of local alternatives defined by

$$K_{(n)}$$
: $\mathbf{H}\boldsymbol{\beta} = \mathbf{h} + \frac{\delta}{\sqrt{n}}$

 $\boldsymbol{\delta} = (\delta_1, \delta_2 \cdots, \delta_q) \in \Re^q$, a real fixed vector.

Note that for $\delta = \mathbf{0}$, $\mathbf{H}\beta = \mathbf{h}$, for all n.

We define a quadratic loss function using a positive definite matrix (p.d.m.) ${\bf Q}$

$$\mathcal{L}(oldsymbol{eta}^*; \mathbf{Q}) = \left[\sqrt{n}(oldsymbol{eta}^* - oldsymbol{eta})
ight]' \mathbf{Q} \left[\sqrt{n}(oldsymbol{eta}^* - oldsymbol{eta})
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Asymptotic Analysis

• The asymptotic distribution function of β^* under $k_{(n)}$ by

$$G(\mathbf{y}) = \lim_{n \to \infty} P\left[\sqrt{n}(\boldsymbol{\beta}^* - \boldsymbol{\beta}) \le \mathbf{y}|k_{(n)}\right],$$

where G(y) is nondegenerate distribution function.

The asymptotic distributional quadratic risk (ADR) by

$$R(\beta^*; \mathbf{Q}) = \int \cdots \int \mathbf{y}' \mathbf{Q} \mathbf{y} dG(\mathbf{y})$$

= trace($\mathbf{Q}\mathbf{Q}^*$)

$$\mathbf{Q}^* = \int \cdots \int \mathbf{y} \mathbf{y}' dG(\mathbf{y})$$

is the dispersion matrix for the distribution G(y).

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Mathematical Proof

Theorem: Under local alternatives $k_{(n)}$ and usual regularity conditions we have the ADB of the proposed estimators as $n \to \infty$ in the following:

$$ADB(\hat{\boldsymbol{\beta}}) = \mathbf{0}, \tag{1}$$

$$ADB(\tilde{\boldsymbol{\beta}}) = -\mathbf{J}\boldsymbol{\delta}, \quad \mathbf{J} = (\mathbf{X}'\mathbf{W}\mathbf{X})^{-1}\mathbf{H}'[\mathbf{H}(\mathbf{X}'\mathbf{W}\mathbf{X})^{-1}\mathbf{H}']^{-1}, \tag{2}$$

$$ADB(\hat{\boldsymbol{\beta}}^{PT}) = \mathbf{J}\delta\Psi_{q+2}(q-2,\Delta), \tag{3}$$

$$ADB(\hat{\boldsymbol{\beta}}^{S}) = -(q-2)\mathbf{J}\delta E(\chi_{q+2}^{-2}(\Delta)), \tag{4}$$

$$ADB(\hat{\boldsymbol{\beta}}^{S^{+}}) = -(q-2)\mathbf{J}\delta\left[E(\chi_{q+2}^{-2}(\Delta)) - E(\chi_{q+2}^{-2}(\Delta)I(\chi_{q+2}^{2}(\Delta) < (q-2)))\right] - \mathbf{J}\delta\Psi_{q+2}(q-2,\Delta),$$
 (5)

The notation $\Psi_{\nu}(q-2,\Delta)$ is the distribution function of non-central chi-square distribution with ν degrees of freedom and non-centrality parameter Δ .

Mathematical Proof

Theorem: Under local alternatives $k_{(n)}$ and usual regularity conditions we have the ADRs of $\hat{\beta}$, $\tilde{\beta}$, $\hat{\beta}^{PT}$, $\hat{\beta}^{S}$ and $\hat{\beta}^{S+}$ are respectively:

$$\begin{split} R(\hat{\beta}) &= & \operatorname{trace}[\mathbf{Q}(\mathbf{X}'\mathbf{W}\mathbf{X})^{-1}], \\ R(\tilde{\beta}) &= & R(\hat{\beta}) - \operatorname{trace}[\mathbf{QJH}(\mathbf{X}'\mathbf{W}\mathbf{X})^{-1}] + \delta'(\mathbf{J}'\mathbf{QJ})\delta, \\ R(\hat{\beta}^{PT}) &= & R(\hat{\beta}) - \operatorname{trace}[\mathbf{QJH}(\mathbf{X}'\mathbf{W}\mathbf{X})^{-1}]\Psi_{q+2}(q-2,\Delta) \\ &+ & \delta'(\mathbf{J}'\mathbf{QJ})\delta[2\Psi_{q+2}(q-2,\Delta) - \Psi_{q+4}(q-2,\Delta)], \\ R(\hat{\beta}^S) &= & R(\hat{\beta}) - 2(q-2)\operatorname{trace}[\mathbf{QJH}(\mathbf{X}'\mathbf{W}\mathbf{X})^{-1}]\{2E(\chi_{q+2}^{-2}(\Delta)) \\ &- & (q-2)E(\chi_{q+2}^{-4}(\Delta))\} + (q-2)\delta'(\mathbf{J}'\mathbf{QJ})\delta\{2E(\chi_{q+2}^{-2}(\Delta)) \\ &- & 2E(\chi_{q+2}^{-4}(\Delta)) + (q-2)E(\chi_{q+4}^{-4}(\Delta))\}, \\ R(\hat{\beta}^{S+}) &= & R(\hat{\beta}^S) - \delta'(\mathbf{J}'\mathbf{QJ})\delta E[(1-(q-2)\chi_{q+4}^{-2}(\Delta))^2I(\chi_{q+4}^2(\Delta) < (q-2))] \\ &- & \operatorname{trace}[\mathbf{QJH}(\mathbf{X}'\mathbf{W}\mathbf{X})^{-1}]E[(1-(q-2)\chi_{q+2}^{-2}(\Delta))^2I(\chi_{q+4}^2(\Delta) < (q-2))] \\ &+ & 2\delta'(\mathbf{J}'\mathbf{QJ})\delta E[(1-(q-2)\chi_{q+4}^{-2}(\Delta))I(\chi_{q+4}^2(\Delta) < (q-2))]. \end{split}$$

- We use Monte Carlo simulation experiments to examine the risk performance of proposed estimators based on large sample methodology under various scenarios.
- Our sampling experiment consists of different combinations of sample sizes, i.e., n = 100, 150, 200.
- In this study we simulate binary response from the following model:

$$\log\left(\frac{p_i}{1-p_i}\right)=\eta_i=\mathbf{x}_i'\boldsymbol{\beta},\quad i=1,\cdots,n,$$

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- For simulation we consider the particular case of hypothesis $H_0: \beta_2 = \mathbf{0}$, where β_2 is a $k_2 \times 1$ vector with $k = k_1 + k_2$.
- We set the true value of β at $\beta = (\beta_1, \beta_2) = (c(1.5, 2.5), \beta_2)$ to generate the binary response y_i .
- The summary of simulation result is provided for $(k_1, k_2) = \{(2, 3), (2, 5), (2, 7)\}$ and $\alpha = 0.05$.
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- ullet The performance of an estimator of eta will be appraised using the mean squared error (MSE) criterion.
- All computations were conducted using the R statistical system (Ihaka and Gentleman, 1996).
- We have numerically calculated the relative MSE of $\tilde{\beta}$, $\hat{\beta}^{PT}$, $\hat{\beta}^{S}$, and $\hat{\beta}^{S+}$ with respect to $\hat{\beta}$ by simulation.
- The simulated relative efficiency (SRE) of the estimator β^{\diamond} to the maximum likelihood estimator $\hat{\beta}$ is denoted by

$$SRE(\hat{\boldsymbol{\beta}}:\boldsymbol{\beta}^{\diamond}) = \frac{MSE(\hat{\boldsymbol{\beta}})}{MSE(\boldsymbol{\beta}^{\diamond})},$$

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- The simulated relative efficiency (SRE) of the estimator β^{\diamond} to the maximum likelihood estimator $\hat{\beta}$ is denoted by

$$\mathsf{SRE}(\hat{\boldsymbol{\beta}}:\boldsymbol{\beta}^\diamond) = \frac{\mathsf{MSE}(\hat{\boldsymbol{\beta}})}{\mathsf{MSE}(\boldsymbol{\beta}^\diamond)},$$

 Keeping in mind that the amount a SRE larger than one indicates the degree of superiority of the estimator β[◊] over β̂.

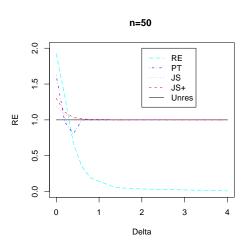


Figure: Relative efficiency of the estimators as a function of non-centrality parameter Δ^* for sample sizes n=150, and insignificant parameters $k_2=3$

Table: Simulated relative MSE with respect to $\hat{\beta}$ for $n = 150, k_2 = 3$.

Δ*	RE	PTE	SE	PSE	
0.0	1.727	1.340	1.153	1.201	
0.2	1.749	1.265	1.147	1.171	
0.4	1.597	1.026	1.105	1.115	
0.6	1.433	0.929	1.069	1.071	
0.8	1.123	0.957	1.053	1.053	
1.0	0.913	0.988	1.046	1.046	
1.2	0.704	0.999	1.042	1.042	
2.0	0.373	1.000	1.032	1.032	
4.0	0.258	1.000	1.024	1.024	

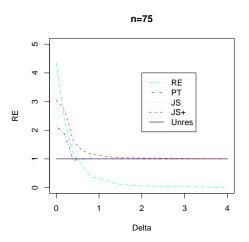


Figure: Relative MSE of the estimators as a function of non-centrality parameter Δ^* for sample sizes n=150, and nuisance parameters $k_2=7$

Table: Simulated relative MSE with respect to $\hat{\beta}$ for $n = 150, k_2 = 7$.

Δ*	RE	PTE	SE	PSE	
0.0	3.184	1.447	1.822	1.926	
0.2	3.020	1.421	1.839	1.912	
0.4	3.061	1.124	1.668	1.709	
0.6	2.680	0.990	1.481	1.488	
0.8	2.058	0.983	1.388	1.391	
1.0	1.716	0.993	1.312	1.313	
1.2	1.352	0.997	1.268	1.268	
2.0	0.739	1.000	1.177	1.177	
4.0	0.572	1.000	1.118	1.118	

Table: Relative efficiency of RE, SE, PSE, L_1 GLM, adaptive L_1 GLM, and SCAD with respect to $\hat{\beta}$ when $\Delta^* = 0$ and n = 200

Method	$k_2 = 3$	$k_2 = 5$	$k_2 = 7$	$k_2 = 11$	$k_2 = 15$	$k_2 = 20$
Restricted	1.79	2.36	3.02	4.50	7.16	9.82
Pretest	1.53	1.81	2.19	2.65	2.67	2.72
Shrinkage	1.16	1.50	1.82	1.63	3.93	4.04
Positive Shrinkage	1.22	1.60	1.98	2.77	4.10	4.28
L_1 GLM	1.24	1.53	1.69	2.51	3.38	3.92
Adaptive L_1 GLM	1.34	1.55	1.77	2.53	3.51	4.02
SCAD	1.51	1.60	1.87	2.61	3.82	4.17

- This data set collected on males in a heart disease high-risk region of western Cape, South Africa.
- A total of 462 individuals are included in this data set.
- The objective of this study was to predict CHD (coronary heart disease)=1 or 0; present or absent, from a set of covariates listed from below:
 - sbp: systolic blood pressure
 - tobacco: cumulative tobacco (kg) IdI: low densiity lipoprotein cholesterol
 - adiposity: Adiposity level of fat tissue
 - famhist: family history of heart disease (Present, Absent)
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Consider the full model

$$log\left(\frac{p_i}{1-p_i}\right) = \beta_0 + \beta_1 \operatorname{sbp}_i + \beta_2 \operatorname{tobacco}_i + \beta_3 \operatorname{Idl}_i + \beta_4 \operatorname{adiposity}_i + \beta_5 \operatorname{famhist}_i + \beta_6 \operatorname{typea}_i + \beta_7 \operatorname{obesity}_i + \beta_8 \operatorname{alcohol}_i + \beta_9 \operatorname{age}_i$$

Table: Estimate (first row) and standard error (second row) for tobacco (β_1) , Idl (β_2) , famhist (β_3) , age (β_4) , and typea (β_5) on coronary heart disease. The SRE column gives the relative efficiency based on bootstrap simulation of the estimators with respect to UE.

Estimators	β_1	β_2	β_3	β_4	β_5	SRE
UE	0.541	0.399	0.190	0.607	0.342	1.0000
	0.284	0.290	0.219	0.352	0.243	
RE	0.506	0.377	0.194	0.699	0.321	2.520
	0.245	0.257	0.204	0.277	0.231	
PT	0.513	0.386	0.194	0.678	0.328	1.476
	0.260	0.273	0.209	0.305	0.225	
SE	0.522	0.391	0.193	0.661	0.332	1.327
	0.265	0.278	0.212	0.322	0.238	
PSE	0.523	0.391	0.192	0.654	0.333	1.547
	0.266	0.275	0.212	0.309	0.237	
L₁GLM	0.407	0.285	0.133	0.538	0.203	1.789
	0.233	0.238	0.162	0.266	0.198	
Adaptive L ₁ GLM	0.407	0.284	0.133	0.538	0.207	1.808
	0.231	0.224	0.164	0.272	0.192	
SCAD	0.387	0.239	0.132	0.483	0.184	1.879
	0.201	0.292	0.156	0.238	0.178	

- Gauss provided two justifications for least squares
 - The maximum likelihood argument in the Gaussian error model.
 - The idea of risk, commonly known as the Gauss-Markov theorem.
- Stein's 1956 paper revealed that neither maximum likelihood estimators nor unbiased estimators have desirable risk functions when the dimension of the parameter space is not small.
- The SE and PSE outperforms the maximum likelihood estimator of the regression parameter vector in the entire parameter space.

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Shrinkage Versus LASSÉ

- The LASSÉ dominates the SE when the number of restrictions on parameters are small.
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