Unit 3

Regularized generalized linear models

Generalized linear models

Introduction

- Linear models are well suited for regression analyses when the response variable is continuous and at least approximately normal.
- In many applications the response is not a continuous variable, but rather binary, categorical, or a count variable.
- Difficulties with linear regression models are also encountered for continuous variables with limited support and which are considerably skewed.
- Generalized linear models (GLMs) unify many regression approaches with response variables that do not necessarily follow a normal distribution.

Binary regression

Binary regression

- Assume that (ungrouped) data on N objects or individuals are given in the form $(y_i, x_{i1}, \ldots, x_{ik})$, $i = 1, \ldots, N$, with the binary response y coded by 0 and 1 and covariates denoted by x_1, \ldots, x_k .
- The covariates x_1, \ldots, x_k may have been derived from an appropriate transformation or coding of the original variables.
- The main goal of a binary regression analysis is then to model and estimate the effects of the covariates on the (conditional) probability

$$\pi_i = \mathsf{P}(y_i = 1 | \mathbf{x}_i) = \mathsf{E}(y_i | \mathbf{x}_i),$$

for the outcome $y_i = 1$ and given values of the covariates $\mathbf{x}_i = (x_{i1}, \dots, x_{ik})^{\top}$.

• The response variables are assumed to be (conditionally) independent.

Linear probability model

The **linear probability model** is given by

$$\pi_i = \beta_0 + \beta_1 x_{i1} + \ldots + \beta_k x_{ik},$$

with linear predictor

$$\eta_i = \beta_0 + \beta_1 \mathbf{x}_{i1} + \ldots + \beta_k \mathbf{x}_{ik} = \mathbf{x}_i^{\top} \boldsymbol{\beta},$$

with
$$\boldsymbol{\beta} = (\beta_0, \beta_1, \dots, \beta_k)^{\top}$$
 and $\boldsymbol{x}_i = (1, x_{i1}, \dots, x_{ik})^{\top}$.

- The linear predictor is equal to the success probability.
- The linear predictor must lie in the interval [0, 1] for all vectors x.
- ullet This requires restrictions on the parameters eta that are difficult to handle in the estimation process.

• Combine the probability π_i with the linear predictor η_i through a relation of the form

$$\pi_i = h(\eta_i) = h(\beta_0 + \beta_1 x_{i1} + \ldots + \beta_k x_{ik}),$$

where h is a strictly monotonically increasing cumulative distribution function on the real line.

- This ensures $h(\eta) \in [0, 1]$.
- In addition one can also write

$$\eta_i = g(\pi_i),$$

with the inverse function $q = h^{-1}$.

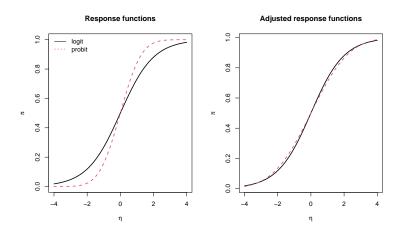
- Within the framework of GLMs, h is called the **response function** and $g = h^{-1}$ is known as the **link function**.
- Logit and probit models are the most widely used binary regression models.

Logit model:

$$\pi = \frac{\exp(\eta)}{1 + \exp(\eta)}$$
 \Leftrightarrow $\log \frac{\pi}{1 - \pi} = \eta.$

Probit model:

$$\pi = \Phi(\eta)$$
 \Leftrightarrow $\phi^{-1}(\pi) = \eta.$



- Instead of the probit one could have used the more general cumulative function h of a N(0, σ^2) distribution with any choice of variance $\sigma^2 \neq 1$.
- Standardizing h yields the relation

$$\pi(\eta) = h(\mathbf{x}^{\top} \boldsymbol{\beta}) = \Phi(\mathbf{x}^{\top} \boldsymbol{\beta} / \sigma) = \Phi(\mathbf{x}^{\top} \tilde{\boldsymbol{\beta}}),$$

where $\tilde{\boldsymbol{\beta}} = \boldsymbol{\beta}/\sigma$.

• The resulting model for the probability $\pi(\eta)$ based on $h(\eta)$ with $\eta = \mathbf{x}^{\top} \boldsymbol{\beta}$ is equivalent to a probit model with the rescaled parameters $\tilde{\boldsymbol{\beta}} = \boldsymbol{\beta}/\sigma$.

- For an adequate comparison of the models, the mean and variance of the CDFs need to be matched.
- The logistic distribution function has variance $\pi^2/3$. Thus it needs to be compared to a rescaled normal distribution whose variance is adjusted to $\sigma^2 = \pi^2/3$.
- The logit and adjusted probit response functions are very similar.
- The estimated coefficients of a logit model differ from the corresponding values of a probit model (with $\sigma^2 = 1$) approximately by the factor $\sigma = \pi/\sqrt{3}$.
- The estimated probabilities $\pi(\eta)$ are very similar.
- This indicates that instead of the absolute values of the (estimated) coefficients rather the ratios should be interpreted.

Binary models and latent linear models

- Binary regression models can be derived by considering a latent (unobserved) continuous response variable.
- The latent variable is connected with the observed binary response via a threshold mechanism.
- Suppose we are investigating the decision of some individuals
 i = 1,..., N when choosing between two alternatives y = 0 and
 y = 1.
- Assume that individuals assign utilities u_{i0} and u_{i1} to each of the two alternatives.
- The alternative that maximizes the utility is chosen, i.e.,

$$y_i = \begin{cases} 1 & u_{i1} > u_{i0}, \\ 0 & u_{i1} \le u_{i0}. \end{cases}$$

Binary models and latent linear models / 2

 Assuming that the unobserved utilities can be additively decomposed and follow a linear model, we obtain

$$u_{i1} = \mathbf{x}_{i}^{\top} \tilde{\boldsymbol{\beta}}_{1} + \tilde{\epsilon}_{i1},$$

 $u_{i0} = \mathbf{x}_{i}^{\top} \tilde{\boldsymbol{\beta}}_{0} + \tilde{\epsilon}_{i0},$

with
$$\mathbf{x}_i = (1, x_{i1}, \dots, x_{ik})^{\top}$$
.

- The unknown coefficient vectors $\tilde{\beta}_1$ and $\tilde{\beta}_0$ determine the effect of the explanatory variables on the utilities.
- The "errors" $\tilde{\epsilon}_{i1}$ and $\tilde{\epsilon}_{i0}$ include the effects of unobserved explanatory variables.

Binary models and latent linear models / 3

Equivalently, we may choose to investigate utility differences

$$\tilde{\mathbf{y}}_i = \mathbf{u}_{i1} - \mathbf{u}_{i0} = \mathbf{x}_i^{\top} (\tilde{\boldsymbol{\beta}}_1 - \tilde{\boldsymbol{\beta}}_0) + \tilde{\epsilon}_{i1} - \tilde{\epsilon}_{i0} = \mathbf{x}_i^{\top} \boldsymbol{\beta} + \epsilon_i,$$
 with $\boldsymbol{\beta} = \tilde{\boldsymbol{\beta}}_1 - \tilde{\boldsymbol{\beta}}_0$ and $\epsilon_i = \tilde{\epsilon}_{i1} - \tilde{\epsilon}_{i0}$.

 Based on this framework, the binary responses y_i follow a Bernoulli distribution with

$$\pi_i = P(y_i = 1 | \mathbf{x}_i) = P(\tilde{y}_i > 0 | \mathbf{x}_i) = P(\mathbf{x}_i^{\top} \boldsymbol{\beta} + \epsilon_i > 0)$$

= $\int I(\mathbf{x}_i^{\top} \boldsymbol{\beta} + \epsilon_i > 0) f(\epsilon_i) d\epsilon_i,$

where $I(\cdot)$ is the indicator function and f is the probability density of ϵ_i .

Binary models and latent linear models / 4

- We obtain different models depending on the choice of *f*:
 - When ϵ_i follows a logistic distribution, we obtain the logit model.
 - When ϵ_i follows a standard normal distribution, we obtain the probit model.

Interpretation of the logit model

Based on the linear predictor

$$\eta_i = \beta_0 + \beta_1 x_{i1} + \ldots + \beta_k x_{ik} = \mathbf{x}_i^{\top} \boldsymbol{\beta},$$

the odds

$$\frac{\pi_i}{1-\pi_i} = \frac{\mathsf{P}(y_i = 1|\mathbf{x}_i)}{\mathsf{P}(y_i = 0|\mathbf{x}_i)}$$

follow the multiplicative model

$$\frac{\mathsf{P}(y_i=1|\mathbf{x}_i)}{\mathsf{P}(y_i=0|\mathbf{x}_i)}=\exp(\beta_0)\cdot\exp(\beta_1x_{i1})\cdot\ldots\cdot\exp(\beta_kx_{ik}).$$

Interpretation of the logit model / 2

If x_{i1} increases by 1 unit to $x_{i1} + 1$, the following changes apply to the relationship of the odds:

$$\frac{P(y_i = 1 | x_{i1} + 1, \ldots)}{P(y_i = 0 | x_{i1} + 1, \ldots)} / \frac{P(y_i = 1 | x_{i1}, \ldots)}{P(y_i = 0 | x_{i1}, \ldots)} = \exp(\beta_1).$$

- $\beta_1 > 0$: $P(y_i = 1)/P(y_i = 0)$ increases,
- $\beta_1 < 0$: $P(y_i = 1)/P(y_i = 0)$ decreases,
- $\beta_1 = 0$: $P(y_i = 1)/P(y_i = 0)$ remains unchanged.

Deviance and deviance residuals

The deviance is defined by

$$D = -2\sum_{i=1}^{N} \{\ell_i(\hat{\mu}_i) - \ell_i(y_i)\}$$

with $\hat{\mu}_i$ are the estimated expectations. $\ell_i(y_i)$ is the log-likelihood of the saturated model where the number of observations is equal to the number of parameters.

The deviance residuals are defined as

$$d_i = \operatorname{sign}(y_i - \hat{y}_i) \sqrt{-2(\ell_i(\hat{\mu}_i) - \ell_i(y_i))}.$$

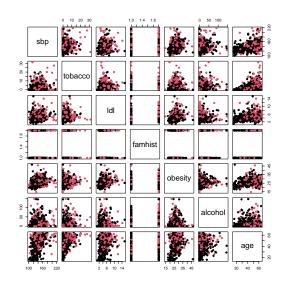
Estimation in R

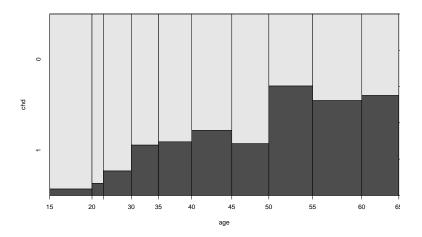
The function for fitting a binary regression model in R is:

```
> glm(formula, family = binomial(link = "logit"), data,
+ weights, subset, na.action, ...)
```

- The formula is specified as for the linear model to model effects on the linear predictor.
- The link for the binomial() family can be specified to be logit, probit or complementary log-log.
- Maximum likelihood estimation is performed using an iterative procedure.

- Data set provided in the R package ElemStatLearn.
- The data set contains 462 observations.
- The dependent variable is chd, an indicator for coronary heart disease.
- The independent variables are the following risk factors:
 - systolic blood pressure (sbp);
 - cumulative tobacco (kg, tobacco);
 - low density lipoprotein cholesterol (1d1);
 - family history of heart disease (famhist);
 - obesity (obesity);
 - current alcohol consumption (alcohol);
 - age at onset (age).





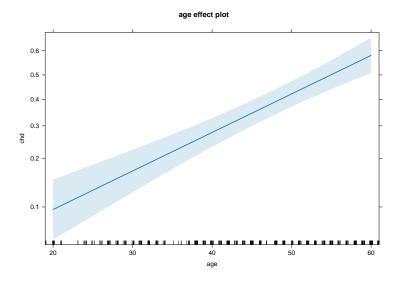
Full logistic regression model:

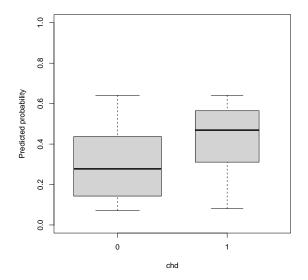
```
> model1 <- glm(chd ~ age, data = SAheart,
+ family = binomial())</pre>
```

```
> summary(model1)
Call:
glm(formula = chd ~ age, family = binomial(), data = SAhear
Coefficients:
           Estimate Std. Error z value Pr(>|z|)
(Intercept) -3.521710  0.416031  -8.465  < 2e-16 ***
        age
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 '
(Dispersion parameter for binomial family taken to be 1)
   Null deviance: 596.11 on 461 degrees of freedom
Residual deviance: 525.56 on 460 degrees of freedom
```

AIC: 529.56

Number of Fisher Scoring iterations: 4





```
> model2 <- glm(chd ~ age + famhist, data = SAheart,</pre>
+ family = binomial())
> model2
Call: glm(formula = chd ~ age + famhist, family = binomial
Coefficients:
   (Intercept)
                          age famhistPresent
      -3.7585
                       0.0597
                                       0.9339
Degrees of Freedom: 461 Total (i.e. Null); 459 Residual
Null Deviance:
                         596.1
Residual Deviance: 506.7
                                AIC: 512.7
```

```
> summary(model2)
Call:
glm(formula = chd ~ age + famhist, family = binomial(), dat
Coefficients:
               Estimate Std. Error z value Pr(>|z|)
(Intercept) -3.758540 0.437062 -8.600 < 2e-16 ***
             0.059705 0.008796 6.787 1.14e-11 ***
age
famhistPresent 0.933937 0.216312 4.318 1.58e-05 ***
               0 '*** 0.001 '** 0.01 '* 0.05 '. '0.1 '
Signif. codes:
(Dispersion parameter for binomial family taken to be 1)
   Null deviance: 596.11 on 461 degrees of freedom
```

Residual deviance: 506.66 on 459 degrees of freedom AIC: 512.66

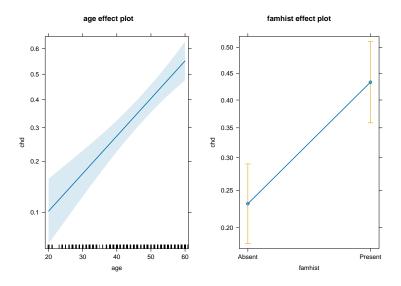
Number of Fisher Scoring iterations: 4

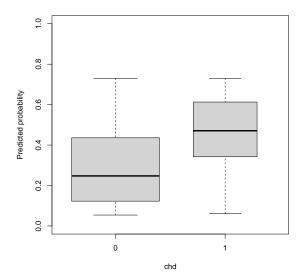
```
> anova(model1, model2)
Analysis of Deviance Table

Model 1: chd ~ age
Model 2: chd ~ age + famhist
   Resid. Df Resid. Dev Df Deviance
1     460     525.56
2     459     506.66     1     18.904
```

```
> anova(model1, model2, test = "Chisq")
Analysis of Deviance Table
Model 1: chd ~ age
Model 2: chd ~ age + famhist
 Resid. Df Resid. Dev Df Deviance Pr(>Chi)
      460 525.56
     459 506.66 1 18.904 1.375e-05 ***
Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 '
```

```
> eff2 <- allEffects(model2)</pre>
> eff2
model: chd ~ age + famhist
age effect
age
       20
                  30
                            40
                                       50
                                                  60
0.1018973 0.1708984 0.2724500 0.4048778 0.5527688
famhist effect
famhist
   Absent Present
0.2310792 0.4333267
```





(Quasi-)complete separation

- Complete separation happens when the outcome variable separates a predictor variable or a combination of predictor variables completely.
- Quasi-complete separation happens when the outcome variable separates a predictor variable or a combination of predictor variables to a certain degree.
- (Quasi-)complete separation leads to large coefficient estimates and standard errors.
- In R no check for (quasi-)complete separation is performed by default. In general issues are indicated by a warning about fitted probabilities being numerically 0 or 1.
- Strategies to deal with (quasi-)complete separation:
 - Assess if the outcome variable is not a dichotomous version of a variable in the model.
 - One might decide not to include the problematic variable in the model. But this may lead to biased estimates.

```
> SAheart0 <- subset(SAheart,
+ (age <= 50 & chd == 0) | (age >= 50 & chd == 1))
> model0 <- glm(chd ~ famhist + age,
+ data = SAheart0, family = binomial())
Warning message:
glm.fit: fitted probabilities numerically 0 or 1 occurred</pre>
```

```
> summary(model0)
Call:
glm(formula = chd ~ famhist + age, family = binomial(), dat
Coefficients:
                Estimate Std. Error z value Pr(>|z|)
(Intercept) -9.526e+02 1.124e+05 -0.008
                                              0.993
famhistPresent 2.877e-01 1.528e+00 0.188
                                              0.851
               1.904e+01 2.249e+03 0.008
                                              0.993
age
(Dispersion parameter for binomial family taken to be 1)
   Null deviance: 399.571 on 324 degrees of freedom
```

on 322

AIC: 16.549

Residual deviance: 10.549

degrees of freedom

Number of Fisher Scoring iterations: 25

Generalized linear regression models

General model definition

The linear model and the regression models for non-normal response variables have common properties that can be summarized in a unified framework:

• The mean $\mu = \mathsf{E}(y)$ of the response y is connected with the linear predictor $\eta = \mathbf{x}^{\top} \boldsymbol{\beta}$ by a response function h or by a link function $g = h^{-1}$:

$$\mu = h(\eta)$$
 or $\eta = g(\mu)$.

The distribution of the response variables (normal, binomial, Poisson, and gamma distribution) can be written in the form of a univariate exponential family.

Univariate exponential families

 The density of a univariate exponential dispersion family for the response variable y is defined by

$$f(y|\theta) = \exp\left(\frac{y\theta - b(\theta)}{a(\phi)} + c(y,\phi)\right).$$

- The parameter θ is called the natural or canonical parameter.
- ullet The second parameter ϕ is a dispersion parameter.
- For the function $b(\theta)$ it is required that $f(y|\theta)$ can be normalized and the first and second derivative $b'(\theta)$ and $b''(\theta)$ exist.
- It can be shown that

$$\mathsf{E}(y) = \mu = b'(\theta), \qquad \mathsf{VAR}(y) = a(\phi)b''(\theta).$$

Univariate exponential families / 2

Examples:

Distribution		$ heta(\mu)$	b(heta)	$\mathit{a}(\phi)$
Normal	$N(\mu, \sigma^2)$	μ	$\theta^2/2$	σ^2
Bernoulli	$B(1,\pi)$	$\log(\pi/(1-\pi))$	$\log(1+\exp(heta))$	1
Poisson	$Po(\lambda)$	$\log(\lambda)$	$\exp(\theta)$	1

Generalized linear model

Distributional assumptions

For given covariates $\mathbf{x}_i = (1, x_{i1}, \dots, x_{ik})^{\top}$, the response variables are (conditionally) independent and the (conditional) density of y_i belongs to the exponential family with

$$f(y_i|\theta_i) = \exp\left(\frac{y_i\theta_i - b(\theta_i)}{a(\phi)} + c(y_i,\phi)\right).$$

The parameter θ_i is called the natural parameter and ϕ the dispersion parameter. For $E(y_i) = \mu_i$ and $VAR(y_i)$, we have

$$\mathsf{E}(y_i) = \mu_i = b'(\theta_i), \qquad \mathsf{VAR}(y_i) = a(\phi)b''(\theta_i).$$

Generalized linear model / 2

Structural assumptions

The (conditional) mean μ_i is connected to the linear predictor $\eta_i = \mathbf{x}_i^{\top} \boldsymbol{\beta} = \beta_0 + \beta_1 \mathbf{x}_{i1} + \ldots + \beta_k \mathbf{x}_{ik}$ through

$$\mu_i = h(\eta_i) = h(\mathbf{x}_i^{\top} \boldsymbol{\beta}), \quad \text{or} \quad \eta_i = g(\mu_i),$$

where

g is a (one-to-one and twice differentiable) response function and h is the link function, i.e., the inverse $g = h^{-1}$.

Maximum likelihood estimation

The ML estimator $\hat{\beta}$ maximizes the (log-)likelihood and is defined as the solution

$$\boldsymbol{s}(\hat{eta})=0$$

of the score function given by

$$\mathbf{s}(oldsymbol{eta}) = \sum_{i=1}^N \mathbf{x}_i rac{h'(\eta_i)}{\mathsf{VAR}(y_i)} (y_i - \mu_i) = \mathbf{X}^ op \mathbf{D} \mathbf{\Sigma}^{-1} (\mathbf{y} - oldsymbol{\mu}),$$

where

Maximum likelihood estimation / 2

The Fisher matrix is

$$F(\beta) = \sum_{i=1}^{N} \mathbf{x}_i \mathbf{x}_i^{\top} \widetilde{\mathbf{w}}_i = \mathbf{X}^{\top} \mathbf{W} \mathbf{X},$$

where

$$\mathbf{W} = \operatorname{diag}(\tilde{w}_1, \dots, \tilde{w}_n)$$

is the diagonal matrix of working weights

$$\tilde{w}_i = \frac{(h'(\eta_i))^2}{\mathsf{VAR}(v_i)}.$$

Maximum likelihood estimation / 3

The ML estimator $\hat{\beta}$ is obtained iteratively using Fisher scoring in form of iteratively weighted least squares estimates

$$\hat{\boldsymbol{\beta}}^{(t+1)} = (\boldsymbol{X}^{\top} \boldsymbol{W}^{(t)} \boldsymbol{X})^{-1} \boldsymbol{X}^{\top} \boldsymbol{W}^{(t)} \tilde{\boldsymbol{y}}^{(t)}, \quad t = 0, 1, 2, \dots,$$

with working observations given by

$$\tilde{y}_i^{(t)} = \hat{\eta}_i^{(t)} + \frac{(y_i - h(\hat{\eta}_i^{(t)}))}{h'(\hat{\eta}_i^{(t)})}.$$

Likelihood inference

Asymptotic properties of the ML estimator

Let $\hat{\beta}_n$ denote the ML estimator based on a sample of size n. Under regularity conditions, $\hat{\beta}_n$ is consistent and asymptotically normal:

$$\hat{\boldsymbol{\beta}}_n \stackrel{a}{\sim} N(\boldsymbol{\beta}, \boldsymbol{F}^{-1}(\boldsymbol{\beta})).$$

This result holds even if the estimator $F(\hat{\beta})$ replaces $F(\beta)$.

Regularized generalized linear models

Regularized GLMs

- Regularized OLS estimation of linear models corresponds to regularized ML estimation.
- The regularized ML criterion can directly be extended to the GLM case.
- The regularized estimator is obtained by solving:

$$\hat{eta}^{\mathsf{pen}} = \operatorname*{arg\,min}_{eta} \left\{ -2\ell(eta, \phi | \mathbf{\emph{y}}, \mathbf{\emph{X}}) + \lambda P(eta)
ight\},$$

where

- twice the negative log-likelihood is used instead of the residual sum of squares;
- the penalty function P() penalizes the "length" of the regression coefficient vector β , e.g., represents the ridge, lasso or elastic net penalty.

Regularized GLMs / 2

- GLMs are usually fitted using iterative weighted least squares (IWLS).
- Estimation of regularized GLMs based on a pathwise coordinate descent algorithm:
 - Compute the solution for a decreasing sequence of penalty parameter values.
 - Initialize coordinate descent algorithm with previous solution.

Software in R

Package **glmnet**:

- Fits a generalized linear model via penalized maximum likelihood.
- The regularization path is computed for the lasso, ridge or elastic net penalty at a grid of values for the regularization parameter λ .
- Implements pathwise coordinate optimization.
- No formula interface is provided.
- By default an intercept is added and the covariates are standardized.

```
Full logistic regression model:
```

```
> full.model <- glm(chd ~ ., data = SAheart,
+ family = binomial())
> printCoefmat(round(coef(summary(full.model)),
+ digits = 2))
```

	Estimate St	d. Error z	value	Pr(> z)	
(Intercept)	-4.13	0.96	-4.28	<2e-16	***
sbp	0.01	0.01	1.02	0.31	
tobacco	0.08	0.03	3.03	<2e-16	***
ldl	0.18	0.06	3.22	<2e-16	***
famhistPresent	0.94	0.22	4.18	<2e-16	***
obesity	-0.03	0.03	-1.19	0.24	
alcohol	0.00	0.00	0.14	0.89	
age	0.04	0.01	4.18	<2e-16	***

Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 '

> step.model <- step(full.model, trace = 0)</pre>

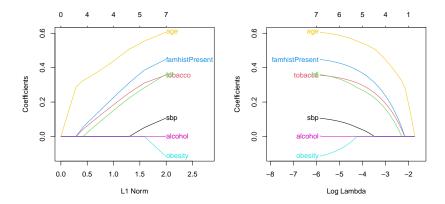
Stepwise selected logistic regression model:

```
> printCoefmat(round(coef(summary(step.model)),
   digits = 2)
+
              Estimate Std. Error z value Pr(>|z|)
(Intercept)
                 -4.20
                             0.50
                                    -8.44 < 2.2e-16 ***
                             0.03
                                     3.16 < 2.2e-16 ***
tobacco
                  0.08
                  0.17
                             0.05
                                     3.09 < 2.2e-16 ***
1d1
famhistPresent
                  0.92
                             0.22
                                     4.14 < 2.2e-16 ***
                             0.01
                  0.04
                                     4.52 < 2.2e-16 ***
age
```

0 '*** 0.001 '** 0.01 '* 0.05 '. ' 0.1 '

Signif. codes:

```
> mf <- model.frame(chd ~ ., data = SAheart)
> X <- model.matrix(chd ~ ., data = mf)[, -1]
> X <- scale(X)
> y <- model.response(mf)
Lasso regression:
> library("glmnet")
> model <- glmnet(X, y, family = "binomial",
+ nlambda = 500)</pre>
```



Ridge regression:

```
> model <- glmnet(X, y, family = "binomial",
+ alpha = 0, nlambda = 500)</pre>
```

