

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 $(y_i, x_{i1}, \dots, x_{ik})$, $i = 1, \dots, N$, with the binary response y coded by 0 and 1 and covariates denoted by x_1, \dots, x_k .
- The covariates x_1, \dots, 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

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

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

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

with linear predictor

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

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

- The linear predictor is equal to the success probability.
- The linear predictor must lie in the interval $[0, 1]$ for all vectors \mathbf{x} .
- This requires restrictions on the parameters $\boldsymbol{\beta}$ that are difficult to handle in the estimation process.

Binary regression models

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

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

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 $g = h^{-1}$.

- 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.

Binary regression models / 2

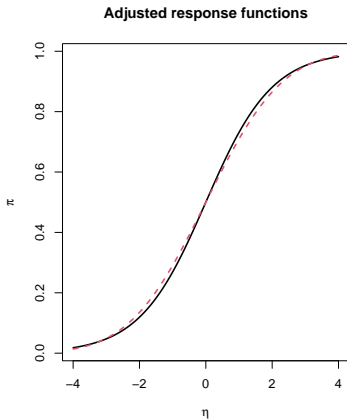
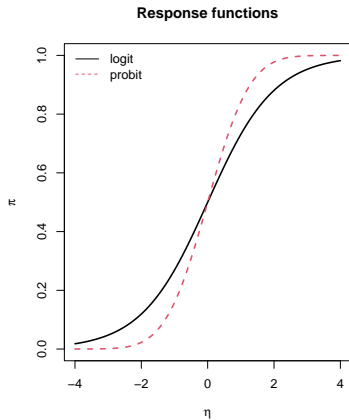
Logit model:

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

Probit model:

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

Binary regression models / 3



Binary regression models / 4

- Instead of the probit one could have used the more general cumulative function h of a $N(0, \sigma^2)$ 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 $\tilde{\boldsymbol{\beta}} = \boldsymbol{\beta} / \sigma$.

Binary regression models / 5

- 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 $i = 1, \dots, N$ 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.,

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

Binary models and latent linear models / 2

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

$$u_{i1} = \mathbf{x}_i^\top \tilde{\beta}_1 + \tilde{\epsilon}_{i1},$$

$$u_{i0} = \mathbf{x}_i^\top \tilde{\beta}_0 + \tilde{\epsilon}_{i0},$$

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

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

with $\beta = \tilde{\beta}_1 - \tilde{\beta}_0$ and $\epsilon_i = \tilde{\epsilon}_{i1} - \tilde{\epsilon}_{i0}$.

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

$$\begin{aligned}\pi_i &= P(y_i = 1 | \mathbf{x}_i) = P(\tilde{y}_i > 0 | \mathbf{x}_i) = P(\mathbf{x}_i^\top \beta + \epsilon_i > 0) \\ &= \int I(\mathbf{x}_i^\top \beta + \epsilon_i > 0) f(\epsilon_i) d\epsilon_i,\end{aligned}$$

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_j follows a logistic distribution, we obtain the logit model.
 - When ϵ_j follows a standard normal distribution, we obtain the probit model.

Interpretation of the logit model

Based on the linear predictor

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

the odds

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

follow the multiplicative model

$$\frac{P(y_i = 1 | \mathbf{x}_i)}{P(y_i = 0 | \mathbf{x}_i)} = \exp(\beta_0) \cdot \exp(\beta_1 x_{i1}) \cdot \dots \cdot \exp(\beta_k x_{ik}).$$

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:

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

- $\beta_1 > 0$: $P(y_i = 1)/P(y_i = 0)$ 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

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

Estimation in R

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

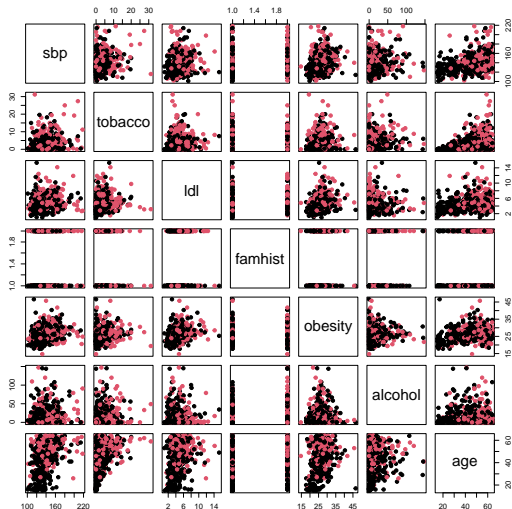
```
> glm(formula, family = binomial(link = "logit"), data,  
+ weights, subset, na.action, ...)
```

- 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.

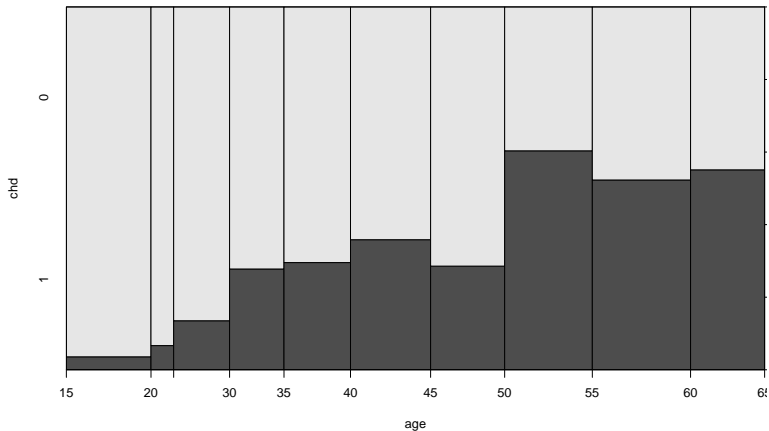
Example: South African Heart Disease

- 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 (`ldl`);
 - family history of heart disease (`famhist`);
 - obesity (`obesity`);
 - current alcohol consumption (`alcohol`);
 - age at onset (`age`).

Example: South African Heart Disease / 2



Example: South African Heart Disease / 3



Example: South African Heart Disease / 4

Full logistic regression model:

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

Example: South African Heart Disease / 5

```
> 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	0.064108	0.008532	7.513	5.76e-14 ***

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

Example: South African Heart Disease / 6

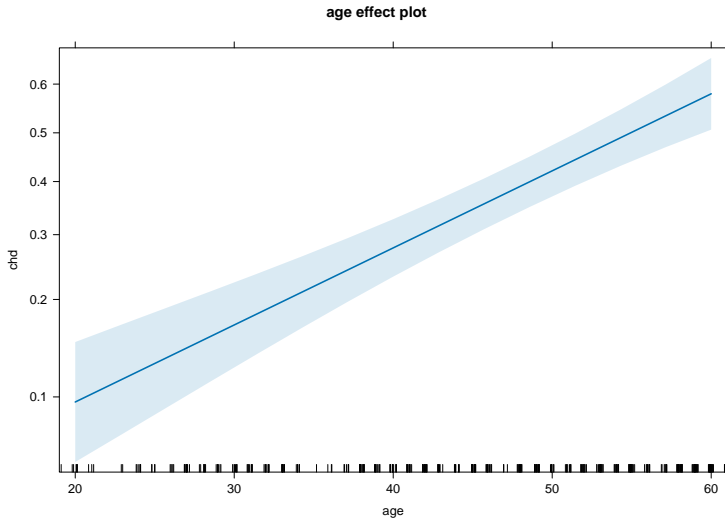
AIC: 529.56

Number of Fisher Scoring iterations: 4

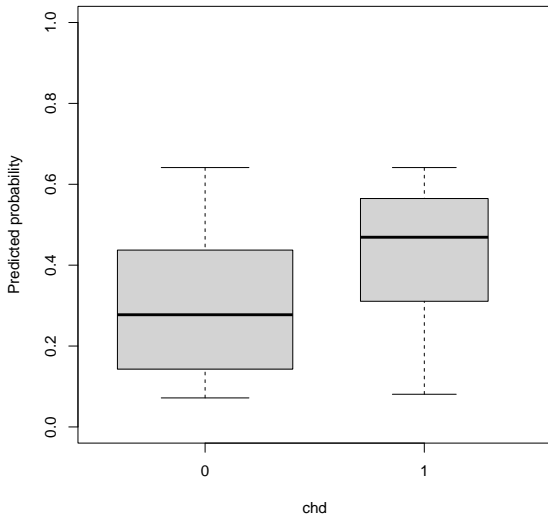
Example: South African Heart Disease / 7

```
> library("effects")
> Effect("age", model1)
  age effect
age
      20      30      40      50      60
0.09625471 0.16819565 0.27740126 0.42157561 0.58048669
> eff1 <- allEffects(model1)
> plot(eff1)
```

Example: South African Heart Disease / 8



Example: South African Heart Disease / 9



Example: South African Heart Disease / 10

```
> model2 <- glm(chd ~ age + famhist, data = SAheart,  
+   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

Example: South African Heart Disease / 11

```
> summary(model2)
```

Call:

```
glm(formula = chd ~ age + famhist, family = binomial(), data = ...)
```

Coefficients:

	Estimate	Std. Error	z value	Pr(> z)	
(Intercept)	-3.758540	0.437062	-8.600	< 2e-16	***
age	0.059705	0.008796	6.787	1.14e-11	***
famhistPresent	0.933937	0.216312	4.318	1.58e-05	***

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

Null deviance: 596.11 on 461 degrees of freedom

Example: South African Heart Disease / 12

Residual deviance: 506.66 on 459 degrees of freedom

AIC: 512.66

Number of Fisher Scoring iterations: 4

Example: South African Heart Disease / 13

```
> anova(model1, model2)
```

```
Analysis of Deviance Table
```

```
Model 1: chd ~ age
```

```
Model 2: chd ~ age + famhist
```

	Resid. Df	Resid. Dev	Df	Deviance	Pr(>Chi)
1	460	525.56			
2	459	506.66	1	18.904	1.375e-05 ***

```
---
```

```
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Example: South African Heart Disease / 14

```
> eff2 <- allEffects(model2)
```

```
> eff2
```

```
model: chd ~ age + famhist
```

```
age effect
```

```
age
```

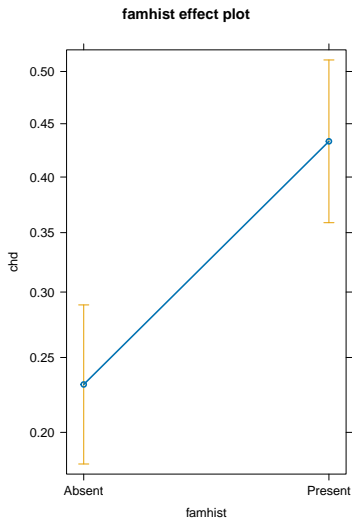
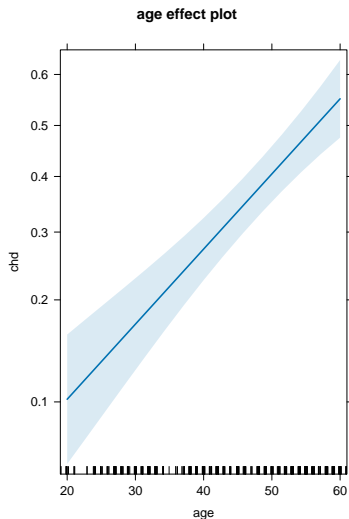
	20	30	40	50	60
	0.1018973	0.1708984	0.2724500	0.4048778	0.5527688

```
famhist effect
```

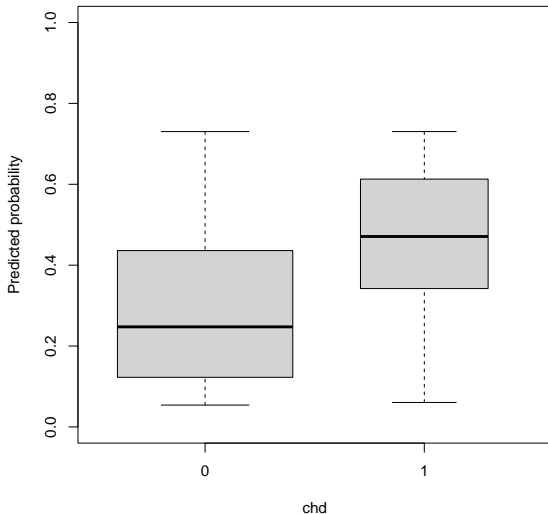
```
famhist
```

	Absent	Present
	0.2310792	0.4333267

Example: South African Heart Disease / 15



Example: South African Heart Disease / 16



(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.

Example: South African Heart Disease

```
> 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

Example: South African Heart Disease / 2

```
> summary(model0)
```

Call:

```
glm(formula = chd ~ famhist + age, family = binomial(), data = 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
age	1.904e+01	2.249e+03	0.008	0.993

(Dispersion parameter for binomial family taken to be 1)

Null deviance: 399.571 on 324 degrees of freedom
Residual deviance: 10.549 on 322 degrees of freedom
AIC: 16.549

Example: South African Heart Disease / 3

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:

- 1 The mean $\mu = E(y)$ 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 $g = h^{-1}$:

$$\mu = h(\eta) \qquad \text{or} \qquad \eta = g(\mu).$$

- 2 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.
- 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

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

Univariate exponential families / 2

Examples:

Distribution		$\theta(\mu)$	$b(\theta)$	$a(\phi)$
Normal	$N(\mu, \sigma^2)$	μ	$\theta^2/2$	σ^2
Bernoulli	$B(1, \pi)$	$\log(\pi/(1 - \pi))$	$\log(1 + \exp(\theta))$	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 $\text{VAR}(y_i)$, we have

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

Generalized linear model / 2

Structural assumptions

The (conditional) mean μ_i is connected to the linear predictor

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

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

where

h is a (one-to-one and twice differentiable) response function and

g 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

$$\mathbf{s}(\hat{\beta}) = 0$$

of the score function given by

$$\mathbf{s}(\beta) = \sum_{i=1}^N \mathbf{x}_i \frac{h'(\eta_i)}{\text{VAR}(y_i)} (y_i - \mu_i) = \mathbf{X}^\top \mathbf{D} \Sigma^{-1} (\mathbf{y} - \boldsymbol{\mu}),$$

where

$$\mathbf{D} = \text{diag}(h'(\eta_1), \dots, h'(\eta_N)), \quad \Sigma = \text{diag}(\text{VAR}(y_1), \dots, \text{VAR}(y_N))$$
$$\boldsymbol{\mu} = (\mu_1, \dots, \mu_N)^\top.$$

Maximum likelihood estimation / 2

The Fisher matrix is

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

where

$$\mathbf{W} = \text{diag}(\tilde{w}_1, \dots, \tilde{w}_N)$$

is the diagonal matrix of working weights

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

Maximum likelihood estimation / 3

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

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

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:

$$\hat{\beta}_N \overset{a}{\sim} N(\beta, \mathbf{F}^{-1}(\beta)).$$

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

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:

$$\hat{\beta}^{\text{pen}} = \arg \min_{\beta} \left\{ -\frac{1}{N} \ell(\beta, \phi | \mathbf{y}, \mathbf{X}) + \lambda P(\beta) \right\},$$

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.

Example: South African Heart Disease

Full logistic regression model:

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

	Estimate	Std. 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	***

Example: South African Heart Disease / 2

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Stepwise selected logistic regression model:

```
> step.model <- step(full.model, trace = 0)
> 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 ***
tobacco	0.08	0.03	3.16	< 2.2e-16 ***
ldl	0.17	0.05	3.09	< 2.2e-16 ***
famhistPresent	0.92	0.22	4.14	< 2.2e-16 ***
age	0.04	0.01	4.52	< 2.2e-16 ***

Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

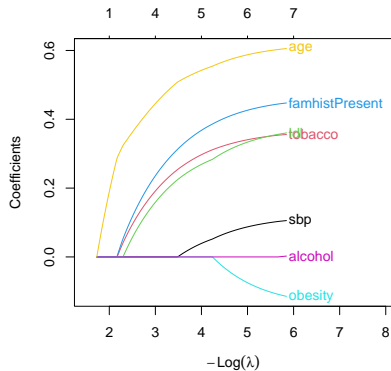
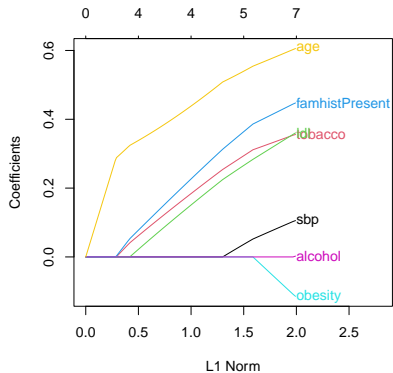
Example: South African Heart Disease / 3

```
> 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)
```

Example: South African Heart Disease / 4



Example: South African Heart Disease / 5

Ridge regression:

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

