Week 3: Generalized Linear Models

MATH-516 Applied Statistics

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Section 1

Introduction

Introduction

- Linear models are only suitable for data that are (approximately) normally distributed
- However, there are many settings where we may wish to analyse a response variable which is not necessarily continuous, including when
- Y is **binary**
- Y is a **count** variable
- Y is **continuous, but non-negative**
- We consider particular distributions for binary/proportion and counts data, in order to do likelihood-based inference

Exponential Family

Definition. The distribution of Y is of exponential type if its density can be written as

$$f(y, \theta, \varphi) = \exp\left(\frac{y\theta - b(\theta)}{\varphi} + c(y, \varphi)\right)$$

where $\theta \in \mathbb{R}$ is the canonical parameter, $\varphi \in (0, \infty)$ is the dispersion parameter, and b, c are real functions

If $b \in C^2$, it can be shown using the moment generating function $m(t) = \mathbb{E}e^{tX}$ that

- $\mu := \mathbb{E}(Y) = b'(\theta)$
- $\mathrm{var}(Y) = \varphi b''(\theta)$
- $\mathrm{var}(Y) = \varphi V(\mu)$, where V is called variance function

Gaussian Distribution

$$f(x, \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right) \quad \text{for} \quad x, \mu \in \mathbb{R} \text{ and } \sigma^2 \in (0, \infty)$$

$$= \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(\frac{x\mu}{\sigma^2} - \frac{\mu^2}{2\sigma^2} - \frac{x^2}{2\sigma^2}\right)$$

$$= \exp\left(\frac{x\mu - \mu^2/2}{\sigma^2} + \left[-\frac{x^2}{2\sigma^2} - \frac{1}{2}\log(2\pi\sigma^2)\right]\right)$$

Hence

- $b(\theta) = \mu^2/2$ and $c(x, \sigma^2) = -\frac{x^2}{2\sigma^2} - \frac{1}{2}\log(2\pi\sigma^2)$ with $\theta = \mu$ and $\varphi = \sigma^2$
- $\text{var}(Y) = \varphi \cdot 1 \Rightarrow V(\mu) \equiv 1$ (variance does not depend on expectation)

Bernoulli Distribution

$$
\begin{aligned}
f(x,p) &= p^x(1-p)^{1-x} \quad \text{for} \quad x \in \{0,1\} \text{ and } p \in (0,1) \\
&= \exp\left\{x \log p + (1-x)\log(1-p)\right\} \\
&= \exp\left\{x \log \frac{p}{1-p} + \log(1-p)\right\}
\end{aligned}
$$

Hence

- $\theta = \log \frac{p}{1-p}$, $\varphi = 1$, $b(\theta) = -\log(1-p)$, and $c(x,\varphi) = 0$
- $\text{var}(Y) = p(1-p)$ and $\mu = \mathbb{E}X = p \Rightarrow V(\mu) = \mu(1-\mu)$

Poisson Distribution

$$f(x) = \frac{\lambda^x}{x!} e^{-\lambda} \quad \text{for} \quad x \in \{0, 1, 2 \ldots\} \text{ and } \lambda \in (0, \infty)$$
$$= \exp\left(x \log \lambda - \lambda + \log(1/x!)\right)$$

Hence

- $\theta = \log \lambda$, $\varphi = 1$, $b(\theta) = e^{\theta}$, and $c(x, \varphi) = \log(1/x!)$
- $\text{var}(Y) = \lambda$ and $\mu = \mathbb{E}X = \lambda \Rightarrow V(\mu) = \mu$

Section 2

GLMs

Generalized Linear Models

- Generalized linear models (GLMs) combine a model for the conditional mean with a distribution (usually within the exponential family) for the response variable and a link function tying predictors and parameters
  - Linear regression (with normal errors) is a special case of a generalized linear model
- Today, we will give an introduction to generalized linear models and focus in particular on binomial regression
  - We will only discuss the case of independent observations
  - Extensions of generalized linear models for correlated and longitudinal (the so-called **generalized linear mixed models**), will be covered in few weeks

Notations

- The starting point is the same as for linear regression:
  - We have a random sample of independent observations

$$(Y_i, \mathrm{X}_{i1}, \ldots, \mathrm{X}_{ip}), \quad i = 1, \ldots, N$$

    where Y is the response variable and $\mathrm{X}_1, \ldots, \mathrm{X}_p$ are p explanatory variables or covariates which are assumed fixed (non-random)

- The goal is to model the response variable as a function of the explanatory variables
- Let μ_i denote the (conditional) mean of Y_i given covariates,

$$\mu_i = \mathbb{E}(Y_i \mid \mathrm{X}_{i1}, \ldots, \mathrm{X}_{ip})$$

- Let η_i denote the linear combination of the covariates that will be used to model the response variable

$$\eta_i = \beta_0 + \beta_1 \mathrm{X}_{i1} + \cdots + \beta_p \mathrm{X}_{ip}$$

Definition

- There are three building blocks to the generalized linear model:
  - A probability distribution for the outcome Y that is a member of the exponential family (normal, binomial, Poisson, gamma, inverse Gaussian, ...)
  - A linear predictor $\eta = \mathbf{X}^\top \beta$
  - A function g, called link function, that links the mean of Y_i to the predictor variables, $g(\mu_i) = \eta_i$
- The link between the mean of Y and the regression "line" is

$$g\left\{\mathbb{E}(Y \mid \mathrm{X}_1, \ldots, \mathrm{X}_p)\right\} = \beta_0 + \beta_1 \mathrm{X}_1 + \cdots + \beta_p \mathrm{X}_p$$

Link Function

- The link function connects the mean to the explanatory variables

$$g(\mu_i) = \eta_i = \beta_0 + \beta_1 \mathrm{X}_{i1} + \cdots + \beta_p \mathrm{X}_{ip}$$
$$\Leftrightarrow \quad \mu_i = g^{-1}(\eta_i) = g^{-1}(\beta_0 + \beta_1 \mathrm{X}_{i1} + \cdots + \beta_p \mathrm{X}_{ip}).$$

- In the ordinary linear regression model, we do not impose constraints on the mean μ_i and $\hat{\mu}_i = \hat{\beta}_0 + \hat{\beta}_1 \mathrm{X}_{i1} + \cdots + \hat{\beta}_p \mathrm{X}_{ip}$ can take on any value in $(-\infty, \infty)$
- For some response variables, we would need to impose constraints on the mean
  - For Bernoulli responses, the mean $\mu = p$ must lie in the interval $(0, 1)$
  - For Poisson responses, the mean λ must be positive
- An appropriate choice of link function sets μ_i equal to a transformation of the linear combination η_i so as to avoid any parameter constraints on β

Choice of Link Function

Certain choices of the link function facilitate interpretation or make the likelihood function convenient for optimization (smooth, i.e., differentiable and monotonic, i.e., invertible)

- For the Bernoulli and binomial distributions, an appropriate link function is the logit function

$$\text{logit}(\mu) := \log\left(\frac{\mu}{1-\mu}\right) = \eta \quad \Leftrightarrow \quad \mu = \frac{\exp(\eta)}{1+\exp(\eta)}$$

- For the Poisson distribution, an appropriate link function is the natural logarithm

$$\log(\mu) = \eta \quad \Leftrightarrow \quad \mu = \exp(\eta)$$

- For the normal distribution, an appropriate link function is the identity function, $\mu = \eta$

MLE in GLM

- $\ell(\beta) = \sum_n \frac{Y_n\theta_n - b(\theta_n)}{\varphi} + c(\varphi, Y_n)$, where
  - $\theta_n = (b')^{-1}(\mu_n)$ and $\mu_n = g^{-1}(\mathbf{X}_n^\top \beta)$

$\Rightarrow$ maximization done via Iteratively Reweighted Least Squares (IRLS) (requires gradient vector and Hessian matrix)

- $U_n(\beta) := \frac{1}{\varphi} w_n g'(\mu_n)(Y_n - \mu_n)X_n$, with $w_n = [V(\mu_n)\{g'(\mu_n)\}^2]^{-1}$
  - shown using the chain and inverse function rules
- Fisher information: $\mathbf{I} = \frac{1}{\varphi}\mathbb{E}(\mathbf{X}^\top \mathbf{W}\mathbf{X})$
  - weight matrix $\mathbf{W}$ diagonal with weights w_n
  - log-likelihood is concave and IRLS converges to the MLE
  - one can work with the Hessian (full Newton) instead of the expected Hessian (Fisher scoring): beware of negative weights!

See Section 3.1 in Wood's book

MLE in GLM

MLE asymptotic theory implies that

- $\hat{\beta} \to \mathcal{N}_p(\beta, \mathbf{I}^{-1})$ [Wald]
  - φ is hidden. If unknown, estimate it consistently and use Cramer-Slutzsky
  - tests for subsets of β are based on the corresponding marginal normal distributions (provided by `summary(glm)` in `R`)
  - used to obtain CIs. Use `confint.default(glm, level=.95)` in `R`
- Let $H_0 : \beta_{p-m+1} = ... = \beta_p = 0$ hold in the GLM, $\hat{\beta}$ denotes parameter estimates in the model, and $\tilde{\beta}$ denotes parameter estimates in the submodel given by the linear constraints in H_0. Then [likelihood ratio]

$$2\{\ell(\hat{\beta}) - \ell(\tilde{\beta})\} \to \chi^2_m$$

  - can only be used when φ is known. Use `car::Anova(glm)` in `R`
  - can be used to get CIs (inverting the acceptance region) and are preferred to Wald's CIs. Use `confint(glm, level=.95)` in `R`

Deviance

Definition

1. The saturated model is a model with the largest possible amount of parameters (i.e., $p = N$ and $\mu_n = y_n$)
2. The statistic $D(\mathbf{Y}, \hat{\beta}) = 2\varphi\{\hat{\ell}(\mathbf{Y}) - \ell(\hat{\beta})\}$, where $\hat{\ell}(\mathbf{Y})$ denotes the maximized log-likelihood of the saturated model, is called the deviance

- it is a goodness-of-fit measure
  - for linear models, it is equal to the residual sum of squares R^2
- it measures the discrepancy in fit between the full and the fitted model and $\varphi^{-1} D(\mathbf{Y}, \hat{\beta}) \sim \chi^2_{N-p-1}$ if the fitted model is adequate ($p + 1$ is the number of β's, including the intercept)
- model `summary(glm)` in `R` provides:
  - null deviance: deviance of the intercept-only model ($N - 1$ df)
  - residual deviance: deviance of the provided model ($N - p - 1$ df)
- can be used for model comparison when φ is unknown (F statistic)

Model Checking: Residuals

- Pearson residuals, a.k.a. standardized residuals

$$\epsilon_n^p = \frac{y_n - \hat{\mu}_n}{\sqrt{V(\hat{\mu}_n)}}$$

  $\Rightarrow$ no trend in mean nor variance when plotted against fitted values
  - departure is proof against linearity
  - are obtained by `residuals(glm, type="pearson")`
  - should have zero mean but distribution can be asymmetric around 0
- Deviance residuals

$$\epsilon_n^d = sign(y_n - \hat{\mu}_n)\sqrt{d_n},$$

  where $D(\mathbf{Y}, \hat{\beta}) = \sum_{n=1}^{N} d_n \Rightarrow$ expected to behave like $\mathcal{N}(0, \varphi)$ (if the model holds)
  - departure is proof against response distribution
  - are obtained by `residuals(glm)` = `residuals(glm, type="deviance")`

See here for examples of model diagnostics

Section 3

Logistic Regression for Bernoulli and Binomial Data

Generalized Linear Model for Binary Variables

- In the case of a binary response variable, assume Y_n follows a Bernoulli distribution with parameter π_n, $Y_n \sim \text{Bin}(\pi_n)$, where

$$\pi_n = \Pr(Y_n = 1 \mid \mathbf{X}_n) = \mathbb{E}(Y_n \mid \mathbf{X}_n)$$

- An appropriate link function for binary responses is the **logit** function

$$g(z) := \text{logit}(z) = \log\left(\frac{z}{1-z}\right)$$

- The **logistic regression model** is

$$g(\pi_n) = \log\left(\frac{\pi_n}{1-\pi_n}\right) = \eta_n := \beta_0 + \beta_1 \mathrm{X}_{n1} + \cdots + \beta_p \mathrm{X}_{np}$$

- The logit function g is the **quantile function of the logistic distribution** and links $\mathbb{E}(Y_n \mid \mathbf{X}_n) = \pi_n(\mathbf{X}_n)$ and η_n

Logistic Regression: Logit Function

- The logistic model is

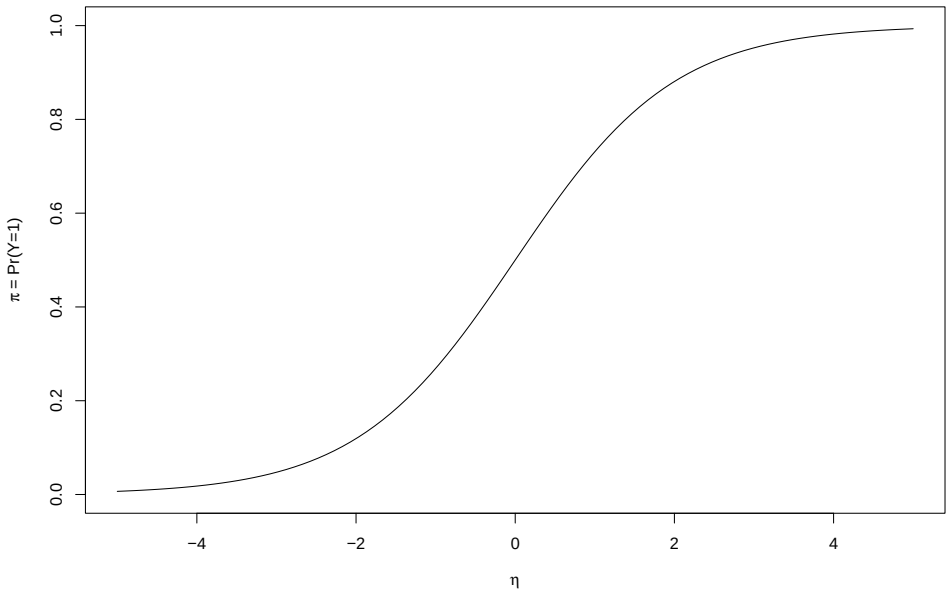
$$\eta_n = \log\left(\frac{\pi_n}{1-\pi_n}\right) = \beta_0 + \beta_1 \mathrm{X}_{n1} + \cdots + \beta_p \mathrm{X}_{np}$$

- This model can also be written on the mean scale by using the inverse-logit function,

$$\mathbb{E}(Y_n \mid \mathbf{X}_n) = \pi_n = \frac{\exp(\beta_0 + \beta_1 \mathrm{X}_{n1} + \cdots + \beta_p \mathrm{X}_{np})}{1 + \exp(\beta_0 + \beta_1 \mathrm{X}_{n1} + \cdots + \beta_p \mathrm{X}_{np})}$$

- We have an expression for the mean $\pi_n = \mathbb{E}(Y_n \mid \mathbf{X}_n)$ as a function of the explanatory variables $\mathbf{X}_n$, but ...
- what does this function look like?
- what does this tell us about the relationship between π_n and η_n (and thus $\mathbf{X}_n$)?

Logistic Distribution Function



- Notice that π is an increasing function of $\eta = \beta_0 + \sum_{j=1}^{p} \beta_j \mathrm{X}_j$
  - If β_j is positive and X_j increases, $\Pr(Y = 1)$ also increases
  - If β_j is negative and X_j increases, $\Pr(Y = 1)$ decreases
- We also see that the relationship between $\Pr(Y = 1)$ and η (and thus each X_j) is non-linear

Parameter interpretations in terms of odds

- Quantifying the effect sizes in logistic regression is not easy because it's a nonlinear model
- The coefficients can be interpreted in terms of **odds** and **odds ratios**
- Let $\pi = \Pr(Y = 1 \mid \mathrm{X}_1, \ldots, \mathrm{X}_p)$, the logistic regression model is

$$\log\left(\frac{\pi}{1-\pi}\right) = \beta_0 + \beta_1 \mathrm{X}_1 + \cdots + \beta_p \mathrm{X}_p$$

- By exponentiating both sides, we obtain

$$\mathrm{odds}(Y \mid \mathbf{X}) = \frac{\pi(\mathbf{X})}{1-\pi(\mathbf{X})} = \exp(\beta_0 + \beta_1 \mathrm{X}_1 + \cdots + \beta_p \mathrm{X}_p),$$

where $\pi(\mathbf{X})/\{1-\pi(\mathbf{X})\}$ are the odds of $\Pr(Y = 1 \mid \mathbf{X})$ relative to $\Pr(Y = 0 \mid \mathbf{X})$

Odds

- The logit function corresponds to modelling the **log-odds**
- The odds for binary Y are the quotient

$$\text{odds}(\pi) = \frac{\pi}{1-\pi} = \frac{\Pr(Y=1)}{\Pr(Y=0)}$$

- For example, an odds of 4 means that the probability that $Y = 1$ is four times higher than the probability that $Y = 0$
- An odds of 0.25 means the probability that $Y = 1$ is only a quarter times the probability that $Y = 0$, or equivalently, the probability that $Y = 0$ is four times higher than the probability that $Y = 1$

$\Pr(Y=1)$	0.1	0.2	0.3	0.4	0.5	0.6	0.7	0.8	0.9
Odds	0.11	0.25	0.43	0.67	1	1.5	2.33	4	9
Odds (frac.)	$\frac{1}{9}$	$\frac{1}{4}$	$\frac{3}{7}$	$\frac{2}{3}$	1	$\frac{3}{2}$	$\frac{7}{3}$	4	9

Interpretation of the intercept in terms of the odds

- When $\mathrm{X}_1 = \cdots = \mathrm{X}_p = 0$, it is clear that

$$\mathrm{odds}(Y \mid \mathbf{X} = \mathbf{0}_p) = \exp(\beta_0)$$

and

$$\Pr(Y = 1 \mid \mathrm{X}_1 = 0, \ldots \mathrm{X}_p = 0) = \frac{\exp(\beta_0)}{1 + \exp(\beta_0)}$$

which represents the probability that $Y = 1$ when $\mathbf{X} = \mathbf{0}_p$

- As for linear regression, $\mathrm{X}_1 = \cdots = \mathrm{X}_p = 0$ might not be physically possible, in which case there is no sensible interpretation for β_0

Parameter interpretation in terms of the odds ratio

Consider for simplicity a logistic model of the form $\text{logit}(\pi) = \beta_0 + \beta_1 x$

The factor $\exp(\beta_1)$ is the change in odds when X increases by one unit,

$$\text{odds}(Y \mid \mathrm{X} = x + 1) = \exp(\beta_1) \times \text{odds}(Y \mid \mathrm{X} = x)$$

- If $\beta_1 = 0$ then the odds ratio is unity
  - meaning that the variable X is not associated with the odds of Y
- If β_1 is positive, then the odds ratio $\exp(\beta_1)$ is larger than one,
  - meaning that, as X increases, the odds of Y increases
- If β_1 is negative, the odds ratio $\exp(\beta_1)$ is smaller than one,
  - meaning that, as X increases, the odds of Y decreases

Interpretation of β_k in terms of odds ratio

For the logistic model, the odds ratio when $\mathrm{X}_k = x_k + 1$ versus $\mathrm{X}_k = x_k$ when $\mathrm{X}_j = x_j$ $(j = 1, \ldots, p, j \neq k)$ is

$$\frac{\text{odds}(Y \mid \mathrm{X}_k = x_k + 1, \mathrm{X}_j = x_j, j \neq k)}{\text{odds}(Y \mid \mathrm{X}_k = x_k, \mathrm{X}_j = x_j, j \neq k)} = \frac{\exp\left(\beta_0 + \sum_{j=1}^{p} \beta_j x_j + \beta_k\right)}{\exp\left(\beta_0 + \sum_{j=1}^{p} \beta_j x_j\right)}$$
$$= \exp(\beta_k)$$

When X_k increases by one unit **and all the other covariates are held constant**, the odds of Y changes by a factor $\exp(\beta_k)$

- The odds increase if $\exp(\beta_k) > 1$, i.e., if $\beta_k > 0$
- The odds decrease if $\exp(\beta_k) < 1$, i.e., if $\beta_k < 0$

Assessing Quality of Fit

The quality of fit of $\hat{\pi}_n$ to y_n (either 0 or 1) is measured by the **deviance**[1]

$$\begin{aligned} \text{Dev}\left(\hat{\pi}_i, y_i\right) &= \begin{cases} -2\log\hat{\pi}_i & \text{if } y_i = 1 \\ -2\log\left(1-\hat{\pi}_i\right) & \text{if } y_i = 0 \end{cases} \\ &= y_i\left(-2\log\hat{\pi}_i\right) + \left(1-y_i\right)\left\{-2\log\left(1-\hat{\pi}_i\right)\right\} \end{aligned}$$

- The Residual Deviance

$$D = \sum_{n=1}^{N} \text{Dev}\left(\hat{\pi}_n, y_n\right)$$

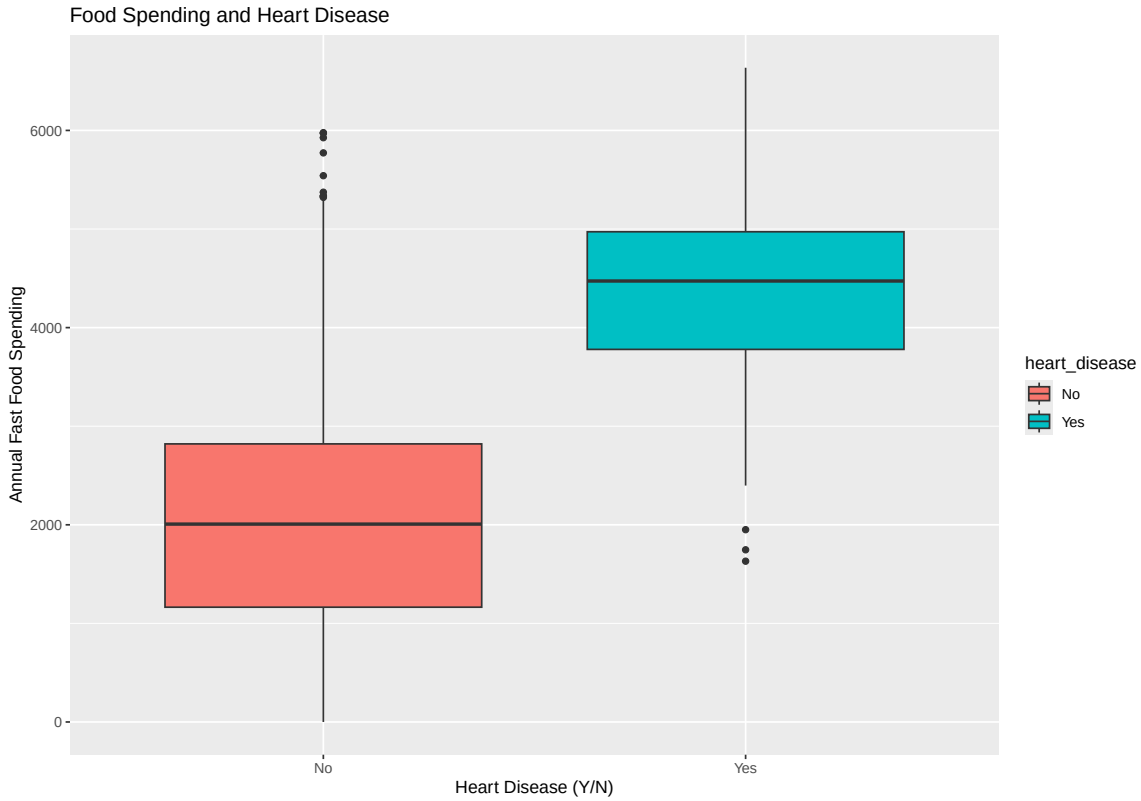
  should behave like χ^2_{N-p-1} if the model is correct **and** n_i's (sample sizes per combination of covariates) are large. ΔD (equiv. LRT) can otherwise be used for model comparison (but not with saturated model)

- The deviance residuals $\epsilon_n^d = sign(y_n - \hat{\pi}_n)\sqrt{\text{Dev}\left(\hat{\pi}_n, y_n\right)}$ have the same interpretation as for the ordinary linear model

[1] the likelihood of the saturated model is 1

Example: Heart Disease Data

Understand how drinking coffee, spending on fast food, and annual income are related to the likelihood of heart disease



Example: Heart Disease Data

```
Call:
glm(formula = factor(heart_disease) ~ factor(coffee_drinker) +
    fast_food_spend + income, family = binomial(link = "logit"),
    data = heart_data)

Coefficients:
                          Estimate Std. Error z value Pr(>|z|)
(Intercept)             -1.087e+01  4.923e-01 -22.080  < 2e-16 ***
factor(coffee_drinker)1 -6.468e-01  2.363e-01  -2.738  0.00619 **
fast_food_spend          2.295e-03  9.276e-05  24.738  < 2e-16 ***
income                   3.033e-06  8.203e-06   0.370  0.71152
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

(Dispersion parameter for binomial family taken to be 1)

    Null deviance: 2920.6  on 9999  degrees of freedom
Residual deviance: 1571.5  on 9996  degrees of freedom
AIC: 1579.5

Number of Fisher Scoring iterations: 8
```

Example: Heart Disease Data

- All covariates except `income` are significant
  - coffee drinking is associated with a decrease in the odds of having a heart disease: a decrease of $\exp(-0.65) \approx 0.52$, ceteris paribus
  - spending in fast food is associated with an increase in the odds of having a heart disease: an increase of $\exp(2.3 * 10^{-3}) \approx 1$, ceteris paribus
- What about predictions?

```
head(predict(log_reg, type="link")) #linear combination of covariates
```

```
        1         2         3         4         5         6
-6.549544 -6.791338 -4.614261 -7.724689 -6.245449 -6.217871
```

```
head(predict(log_reg, type="response")) #predicted probabilities
```

```
           1            2            3            4            5            6
0.0014287239 0.0011222039 0.0098122716 0.0004415893 0.0019355062 0.0019895182
```

Example: Heart Disease Data

What about binary classification?

Once you have predicted probabilities, how large should a predicted probability be to predict a heart disease?

- a cutoff of 0.5 seems a fair choice, but why?
  - it estimates the Bayes Classifier

$$\mathcal{C}_{Bayes}(\mathbf{x}) = \underset{0 \leq k \leq J-1}{\arg\max} \Pr(Y = k | \mathbf{X} = \mathbf{x})$$

- would a cutoff of 0.55 be better?

Section 4

Classification and Model Evaluation

Confusion Matrix

Given any chosen cutoff c, we can form binary predictions for each observation by applying the cutoff to the fitted probabilities

$$\hat{y}_i = \begin{cases} 1 & \text{if } \hat{\pi}_i > c \\ 0 & \text{if } \hat{\pi}_i \leq c \end{cases}$$

The **confusion matrix**

	$\hat{y} = 0$	$\hat{y} = 1$	
$y = 0$	# true negative (TN)	# false positive (FP)	N_0
$y = 1$	# false negative (FN)	# true positive (TP)	N_1

- the diagonal gives the count of the correctly predicted instances

$$accuracy = (\#TP + \#TN)/(N_0 + N_1)$$

$\Rightarrow$ an optimal cutoff can be chosen to minimize $\#FP + \#FN$ or (equivalently) maximize accuracy of the classifier. But not always ...

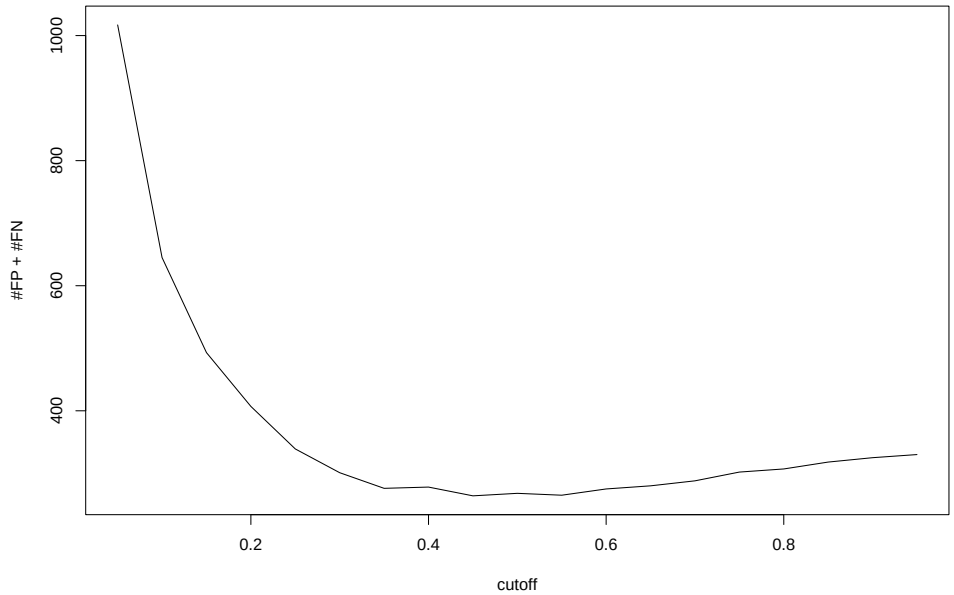
Heart Disease Data: Confusion Matrix

Table 2: cutoff 0.5 - accuracy=0.9732

	0	1
0	9627	40
1	228	105

Table 3: cutoff 0.35 - accuracy=0.9724

	0	1
0	9571	96
1	180	153



The smallest value corresponds to the cutoff 0.55. **Remember to check accuracy on a test set (out of sample)**

ROC curves [2]

Let's define two measures of performance

- Sensitivity = true positive rate = $\#TP/N_1$
  - sensitivity decreases as the cutoff increases
- Specificity = true negative rate = $\#TN/N_0$ = 1-FPR
  - specificity increases as the cutoff increases

Accuracy can be misleading if one class appears much more frequently than another, as in the Heart Disease dataset

- a model that just blindly predicts all patients to not develop heart disease would achieve an accuracy of 96.67%
- the accuracy would be even higher under more extreme imbalance (very rare disease)

$\Rightarrow$ To compare classifiers across all cutoffs, we look at the ROC (Receiver Operating Characteristics) curve

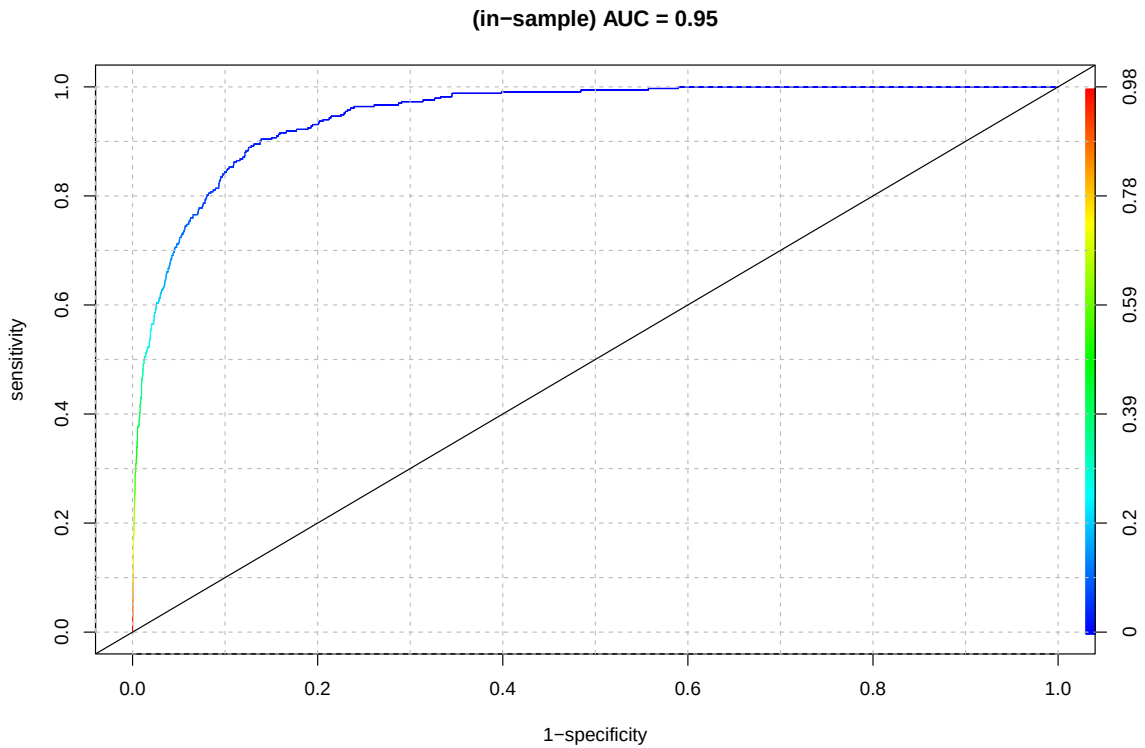
[2] Wojtek J. Krzanowski and David J. Hand, ROC Curves for Continuous Data (2009)

ROC curve

If the purpose of the logistic regression is to construct a predictive model, then a ROC curve is a useful graphical assessment of fit

- ROC curve plots the specificity against $1-$sensitivity for a range of cutoffs $\rightarrow$ takes the trade-off between FP and TP into account
- a coin-toss classifier $\equiv$ ROC curve is identity
- the area under the curve (AUC) is a measure of prediction accuracy
  - the larger the AUC, and hence the farther away the ROC curve is from the diagonal, the better the model performance
  - the AUC has also a probabilistic interpretation (see, e.g., Pepe, 2003, p. 78): It is is the probability that the real-valued model output (e.g., the probability) for a randomly selected `Yes` case will be higher than the real-valued model output for a randomly selected `No` case
- computing AUC allows to quantitatively evaluate model performance
  - this could serve as a useful tool for model comparison as well
  - AUC$=1 \Rightarrow$ model perfectly distinguishes between positive and negative
  - AUC$=0.5 \Rightarrow$ model is no better than a random classifier

Heart Disease: ROC curve



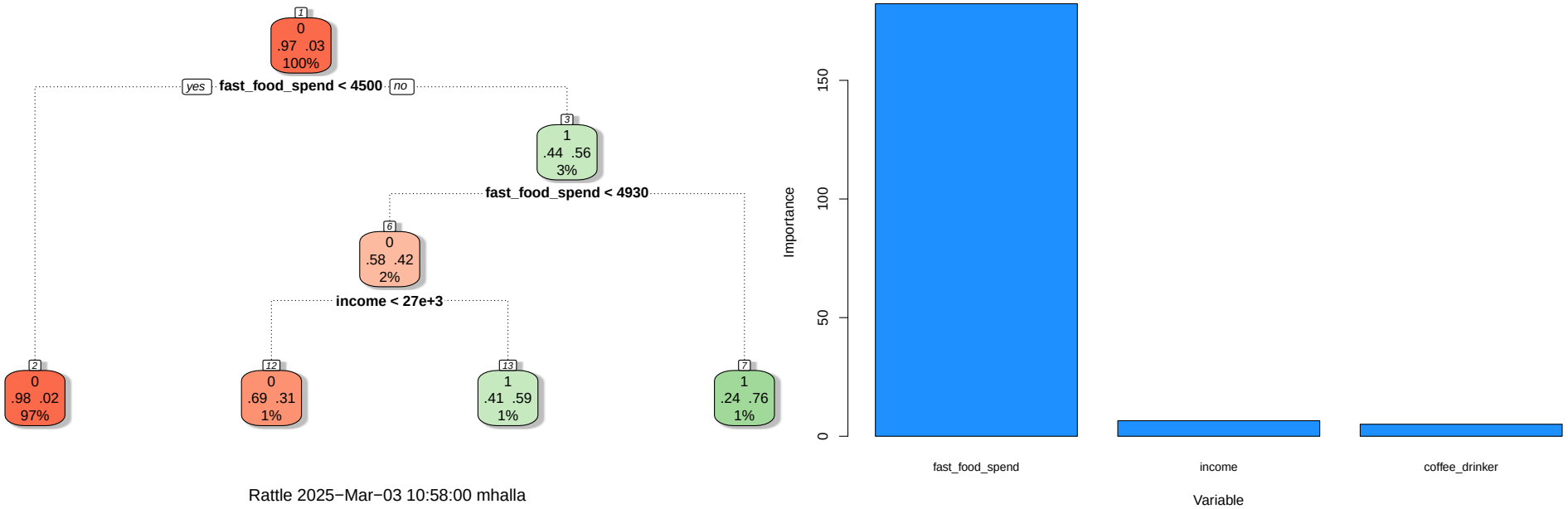
A good model has a high AUC, i.e., as often as possible a high sensitivity and specificity!

Note: AUC should be estimated out-of-sample or cross-validated (AUC= 0.9497 with 5 folds)

Heart Disease: Classification Tree [3]

```
library(rpart)
library(rattle)

tree <- rpart(heart_disease ~., data=heart_data, method="class")
fancyRpartPlot(tree,palettes=c("Reds", "Greens"))
VI <- tree$variable.importance
barplot(VI, xlab="Variable", ylab="Importance", names.arg=names(VI),cex.names=0.8,
```



[3] See the MATH-517 lecture notes

Heart Disease: Classification Tree

What about prediction and accuracy?

```
ConfusionMatrix <- predict(tree, heart_data, type="class")
matrix          <- table(heart_data$heart_disease,ConfusionMatrix)
print(matrix)
```

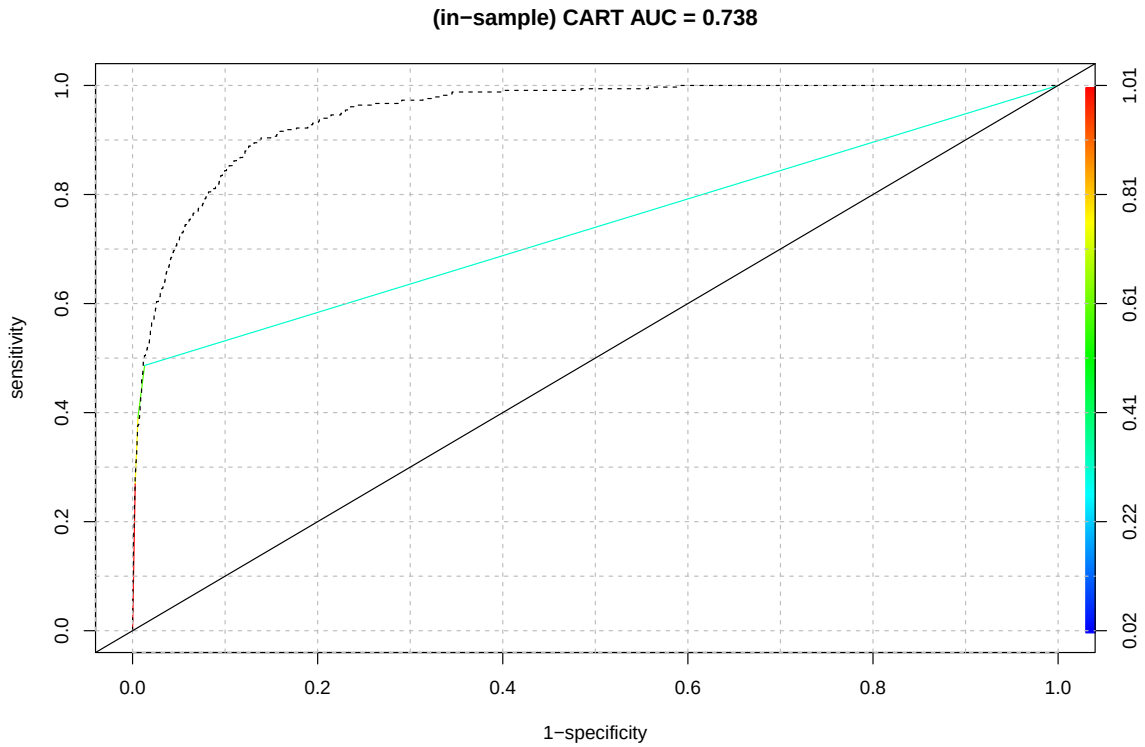
```
   ConfusionMatrix
       0    1
  0 9611   56
  1  203  130
```

```
accuracy <- sum(diag(matrix))/sum(matrix)
print(accuracy)
```

```
[1] 0.9741
```

Heart Disease: Classification Tree

Since classification is binary with decision trees, one can use predicted class probabilities to construct a ROC curve



Classification: Final Remarks

- A classifier assumes a model for the joint distribution of $(Y, \mathbf{X})$ and estimates it
  - Naive Bayes estimates a likelihood and a prior ($\Pr(\mathbf{X} \mid Y) \Pr(Y)$) based on assumptions of conditional independencies
  - Logistic regression estimates $\Pr(Y \mid \mathbf{X})$ parametrically
  - Classification trees estimate $\Pr(Y \mid \mathbf{X})$ non-parametrically
- Criteria for a good classifier
  - Accuracy (report AUC as it works under imbalance)
  - Runtime
  - Interpretability
  - Flexibility

Section 5

General Tips

How to approach an analysis?

It is not possible/desirable to produce a recipe that works for all analyses, but here are some guidelines

1. Always start by identifying the questions that you are trying to answer by analysing the data
2. Always look at the data before fitting any model. Plot the data to get a feel of how variables are related. Check for obvious errors. If you can think of simple methods (plots) that will give you informal answers to your questions, use them before starting the formal model based analysis
3. Now think about how you can use statistical methods/models to answer the questions of interest
4. Once you start fitting the models that are part of your analysis, make sure that you check that the modelling assumptions are met
5. Always make sure that you interpret the results of your modelling in terms of the original question, and think carefully about any limitations that apply to the answer

Some principles for writing up a statistical analysis

1. Always clearly explain the context, and the questions being addressed
2. Make sure that your analysis is repeatable by any statistician with access to the data, using the software of their choice. This means presenting models and results in universal mathematical language, not as `R` code and output
3. Always explain the 'why' of your analysis as well as the 'what'
4. Relate your conclusions back to the questions, and be careful to discuss the limitations of the approach taken
5. Aim to be concise and useful