

Analysis of ordinal data with cumulative link models —
estimation with the **R**-package **ordinal**

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1 Introduction

Ordered categorical data, or simply *ordinal* data, are commonplace in scientific disciplines where humans are used as measurement instruments. Examples include school gradings, ratings of preference in consumer studies, degree of tumor involvement in MR images and animal fitness in field ecology. Cumulative link models are a powerful model class for such data since observations are treated rightfully as categorical, the ordered nature is exploited and the flexible regression framework allows in-depth analyses.

The name *cumulative link models* is adopted from Agresti (2002), but the models are also known as *ordinal regression models* although that term is sometimes also used for other regression models for ordinal responses such as *continuation ratio models* (see e.g., Agresti, 2002). Other aliases are *ordered logit models* and *ordered probit models* (Greene and Hensher, 2010) for the logit and probit link functions. Further, the cumulative link model with a logit link is widely known as the *proportional odds model* due to McCullagh (1980), also with a complementary log-log link, the model is known as *proportional hazards model* for grouped survival times.

Ordinal response variables can be analyzed with omnibus Pearson χ^2 tests, base-line logit models or log-linear models. This corresponds to assuming that the response variable is nominal and information about the ordering of the categories will be ignored. Alternatively numbers can be attached to the response categories, e.g., $1, 2, \dots, J$ and the resulting scores can be analyzed by conventional linear regression and ANOVA models. This approach is in a sense over-confident since the data are assumed to contain more information than they actually do. Observations on an ordinal scale are classified in ordered categories, but the distance between the categories is generally unknown. By using linear models the choice of scoring impose assumptions about the distance between the response categories. Further, standard errors and tests from linear models rest on the assumption that the response, conditional on the explanatory variables, is normally distributed (equivalently the residuals are assumed to be normally distributed). This cannot be the case since the scores are discrete and responses beyond the end categories are not possible. If there are many responses in the end categories, there will most likely be variance heterogeneity to which F and t tests can be rather sensitive. If there are many response categories and the response does not pile up in the end categories, we may expect tests from linear models to be accurate enough, but any bias and optimism is hard to quantify.

Cumulative link models provide the regression framework familiar from linear models while treating the response rightfully as categorical. While cumulative link models are not the only type of ordinal regression model, they are by far the most popular class of ordinal regression models.

Common to the application of methods for nominal responses and linear models to ordinal responses is that interpretation of effects on the ordinal response scale is awkward. For example, linear models will eventually give predictions outside the possible range and statements such as “the response increase 1.2 units with each degree increase in temperature” will only be approximately valid in a restricted range of the response variable.

In this document cumulative link models are described for modeling ordinal response variables. We also describe these models are fitted and data are analyzed with the functionality provided in the `ordinal` package for R (R Development Core Team, 2011).

Example 1 (The wine data): As an example of the data set with an ordinal response variable

Table 1: Wine data from Randall (1989).

Temperature	Contact	Least—Most bitter				
		1	2	3	4	5
cold	no	4	9	5	0	0
cold	yes	1	7	8	2	0
warm	no	0	5	8	3	2
warm	yes	0	1	5	7	5

consider the wine data from Randall (1989) available in the object `wine` in package `ordinal`, cf. Table 1. The data represent a factorial experiment on factors determining the bitterness of wine with 1 = “least bitter” and 5 = “most bitter”. Two treatment factors (temperature and contact) each have two levels. Temperature and contact between juice and skins can be controlled when crushing grapes during wine production. Nine judges each assessed wine from two bottles from each of the four treatment conditions, hence there are 72 observations in all. In Table 1 we have aggregated data over bottles and judges for simplicity, but these variables will be considered later. Initially we only assume that, say, category 4 is larger than 3, but not that the distance between 2 and 3 is half the distance between 2 and 4, for example. The main objective is to examine the effect of contact and temperature on the perceived bitterness of wine. \square

2 Cumulative link models

A cumulative link model is a model for an ordinal response variable, Y_i that can fall in $j = 1, \dots, J$ categories.¹ Then Y_i follows a multinomial distribution with parameter $\boldsymbol{\pi}$ where π_{ij} denote the probability that the i th observation falls in response category j . We define the cumulative probabilities as²

$$\gamma_{ij} = P(Y_i \leq j) = \pi_{i1} + \dots + \pi_{ij} . \quad (1)$$

Initially we will consider the logit link. The logit function is defined as $\text{logit}(\pi) = \log[\pi/(1 - \pi)]$ and cumulative logits are defined as:

$$\text{logit}(\gamma_{ij}) = \text{logit}(P(Y_i \leq j)) = \log \frac{P(Y_i \leq j)}{1 - P(Y_i \leq j)} \quad j = 1, \dots, J - 1 \quad (2)$$

so that the cumulative logits are defined for all but the last category.³

A cumulative link model with a logit link, or simply *cumulative logit model* is a regression model for cumulative logits:

$$\text{logit}(\gamma_{ij}) = \theta_j - \mathbf{x}_i^T \boldsymbol{\beta} \quad (3)$$

where \mathbf{x}_i is a vector of explanatory variables for the i th observation and $\boldsymbol{\beta}$ is the corresponding set of regression parameters. The $\{\theta_j\}$ parameters provide each cumulative logit (for each j) with its own intercept. A key point is that the regression part $\mathbf{x}_i^T \boldsymbol{\beta}$ is independent of j , so $\boldsymbol{\beta}$ has the same effect for each of the $J - 1$ cumulative logits. Note that $\mathbf{x}_i^T \boldsymbol{\beta}$ does

¹where $J \geq 2$. If $J = 2$ binomial models also apply, and in fact the cumulative link model is in this situation identical to a generalized linear model for a binomial response.

²we have suppressed the conditioning on the covariate vector, \mathbf{x}_i , so we have that $\gamma_{ij} = \gamma_j(\mathbf{x}_i)$ and $P(Y_i \leq j) = P(Y \leq j | \mathbf{x}_i)$.

³since for $j = J$ the denominator would be $1 - P(Y_i \leq J) = 1 - 1 = 0$ and thus the fraction is not defined.

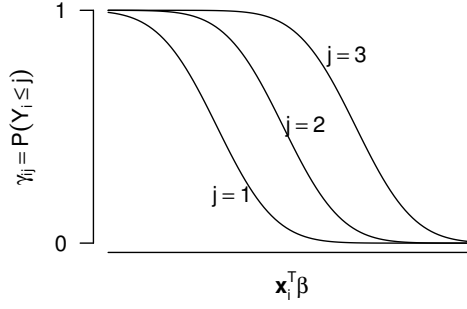


Figure 1: Illustration of a cumulative link model with four response categories.

Table 2: Estimates from ordinary logistic regression models (OLR) and a cumulative logit model (CLM) fitted to the wine data (cf. Table 1).

j	OLR		CLM	
	Intercept	contact	θ_j	contact
1	-2.08	-1.48(1.14)	-2.14	1.21(0.45)
2	0.00	-1.10(0.51)	0.04	
3	1.82	-1.37(0.59)	1.71	
4	2.83	-1.01(0.87)	2.98	

not contain an intercept, since the $\{\theta_j\}$ act as intercepts. The cumulative logit model is illustrated in Fig. 1 for data with four response categories. For small values of $\mathbf{x}_i^T \boldsymbol{\beta}$ the response is likely to fall in the first category and for large values of $\mathbf{x}_i^T \boldsymbol{\beta}$ the response is likely to fall in the last category. The horizontal displacements of the curves are given by the values of $\{\theta_j\}$.

Some sources write the cumulative logit model, (3) with a plus on the right-hand-side, but there are two good reasons for the minus. First, it means that the larger the value of $\mathbf{x}_i^T \boldsymbol{\beta}$, the higher the probability of the response falling in a category at the upper end of the response scale. Thus $\boldsymbol{\beta}$ has the same direction of effect as the regression parameter in an ordinary linear regression or ANOVA model. The second reason is related to the latent variable interpretation of cumulative link models that we will consider in section 2.6.

Example 2: We will consider a cumulative logit model for the wine data including an effect of contact. The response variable is the bitterness ratings, thus each y_i takes a value from 1 to 5 representing the degree of bitterness for the i th sample. We may write the cumulative logit model as:

$$\text{logit}(\gamma_{ij}) = \theta_j - \beta_2(\text{contact}_i), \quad j = 1, \dots, 4, \quad i = 1, \dots, 72.$$

The parameter estimates are given in the last two columns of Table 2. If we consider the cumulative logit model (3) for a fixed j , e.g., for $j = 1$, then the model is just a ordinary logistic regression model where the binomial response is divided into those observations falling in category j or less ($Y_i \leq j$), and those falling in a higher category than j ($Y_i > j$). An initial analysis might indeed start by fitting such an ordinary logistic regression models for a dichotomized response. If we proceed in this vein, we could fit the $J - 1 = 4$ ordinary logistic regression model by fixing j at 1, 2, 3, and 4 in turn. The estimates of those four ordinary

logistic regression models are given in Table 2 under the OLR heading. The cumulative logit model can be seen as the model that combines these four ordinary logistic regression models into a single model and therefore makes better use of the information in the data. A part from a sign difference the estimate of the effect of `contact` from the cumulative logit model is about the average of the `contact` effect estimates from the ordinary logistic regression models. Also observe that the standard error of the `contact` effect is smaller in the cumulative logit model than in any of the ordinary logistic regression models reflecting that the effect of `contact` is more accurately determined in the cumulative logit model. The intercepts from the ordinary logistic regression models are also seen to correspond to the threshold parameters in the cumulative logit model.

The four ordinary logistic regression models can be combined in a single ordinary logistic regression model providing an even better approximation to the cumulative link model. This is considered further in Appendix A. \square

2.1 Fitting cumulative link models with `clm` from package `ordinal`

Cumulative link models can be fitted with `clm` from package `ordinal`. The function takes the following arguments:

```
function (formula, scale, nominal, data, weights, start, subset, doFit = TRUE,
  na.action, contrasts, model = TRUE, control = list(), link = c("logit",
    "probit", "cloglog", "loglog", "cauchit", "Aranda-Ordaz",
    "log-gamma"), threshold = c("flexible", "symmetric", "symmetric2",
    "equidistant"), ...)
```

Most arguments are standard and well-known from `lm` and `glm`, so they will not be introduced. The `formula` argument is of the form `response ~ covariates` and specifies the linear predictor. The `response` should be an *ordered factor* (see `help(factor)`) with levels corresponding to the response categories. A number of link functions are available and the logit link is the default. The `doFit` and `threshold` arguments will be introduced in later sections. For further information about the arguments see the help page for `clm`⁴.

Example 3: In this example we fit a cumulative logit model to the wine data presented in example 1 with `clm` from package `ordinal`. A cumulative logit model that includes additive effects of temperature and contact is fitted and summarized with

```
> fm1 <- clm(rating ~ contact + temp, data = wine)
> summary(fm1)

formula: rating ~ contact + temp
data:      wine

link threshold nobs logLik AIC      niter max.grad cond.H
logit flexible  72   -86.49 184.98 6(0)  4.01e-12 2.7e+01

Coefficients:
              Estimate Std. Error z value Pr(>|z|)
contactyes    1.5278      0.4766   3.205  0.00135 **
tempwarm      2.5031      0.5287   4.735  2.19e-06 ***
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

⁴Typing `?clm` or `help(clm)` in the command prompt should display the help page for `clm`.

Threshold coefficients:

	Estimate	Std. Error	z value
1 2	-1.3444	0.5171	-2.600
2 3	1.2508	0.4379	2.857
3 4	3.4669	0.5978	5.800
4 5	5.0064	0.7309	6.850

The summary provides basic information about the model fit. There are two coefficient tables: one for the regression variables and one for the thresholds or cut-points. Often the thresholds are not of primary interest, but they are an integral part of the model. It is not relevant to test whether the thresholds are equal to zero, so no p -values are provided for this test. The condition number of the Hessian is a measure of how identifiable the model is; large values, say larger than $1e4$ indicate that the model may be ill defined. From this model it appears that contact and high temperature both lead to higher probabilities of observations in the high categories as we would also expect from examining Table 1.

The Wald tests provided by `summary` indicate that both contact and temperature effects are strong. More accurate likelihood ratio tests can be obtained using the `drop1` and `add1` methods (equivalently `dropterm` or `addterm`). The Wald tests are marginal tests so the test of e.g., `temp` is measuring the effect of temperature while *controlling* for the effect of contact. The equivalent likelihood ratio tests are provided by the `drop`-methods:

```
> drop1(fm1, test = "Chi")
```

Single term deletions

Model:

```
rating ~ contact + temp
      Df    AIC    LRT Pr(>Chi)
<none>    184.98
contact  1 194.03 11.043 0.0008902 ***
temp     1 209.91 26.928 2.112e-07 ***
---
```

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

In this case the likelihood ratio tests are slightly more significant than the Wald tests. We could also have tested the effect of the variables while *ignoring* the effect of the other variable. For this test we use the `add`-methods:

```
> fm0 <- clm(rating ~ 1, data = wine)
> add1(fm0, scope = ~ contact + temp, test = "Chi")
```

Single term additions

Model:

```
rating ~ 1
      Df    AIC    LRT Pr(>Chi)
<none>    215.44
contact  1 209.91  7.5263  0.00608 **
temp     1 194.03 23.4113 1.308e-06 ***
---
```

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

where we used the `scope` argument to indicate which terms to include in the model formula. These tests are a little less significant than the tests controlling for the effect of the other variable.

Conventional symmetric so-called Wald confidence intervals for the parameters are available as

```
> confint(fm1, type = "Wald")
```

	2.5 %	97.5 %
1 2	-2.3578848	-0.330882
2 3	0.3925794	2.109038
3 4	2.2952980	4.638476
4 5	3.5738541	6.438954
contactyes	0.5936345	2.461961
tempwarm	1.4669081	3.539296

More accurate profile likelihood confidence intervals are also available and these are discussed in section 4. \square

2.2 Odds ratios and proportional odds

The odds ratio of the event $Y \leq j$ at \mathbf{x}_1 relative to the same event at \mathbf{x}_2 is

$$\text{OR} = \frac{\gamma_j(\mathbf{x}_1)/[1 - \gamma_j(\mathbf{x}_1)]}{\gamma_j(\mathbf{x}_2)/[1 - \gamma_j(\mathbf{x}_2)]} = \frac{\exp(\theta_j - \mathbf{x}_1^T \boldsymbol{\beta})}{\exp(\theta_j - \mathbf{x}_2^T \boldsymbol{\beta})} = \exp[(\mathbf{x}_2^T - \mathbf{x}_1^T) \boldsymbol{\beta}]$$

which is independent of j . Thus the cumulative odds ratio is proportional to the distance between \mathbf{x}_1 and \mathbf{x}_2 which made McCullagh (1980) call the cumulative logit model a *proportional odds model*. If x represent a treatment variable with two levels (e.g., placebo and treatment), then $x_2 - x_1 = 1$ and the odds ratio is $\exp(-\beta_{\text{treatment}})$. Similarly the odds ratio of the event $Y \geq j$ is $\exp(\beta_{\text{treatment}})$.

Confidence intervals for the odds ratios are obtained by transforming the limits of confidence intervals for $\boldsymbol{\beta}$, which will lead to asymmetric confidence intervals for the odds ratios. Symmetric confidence intervals constructed from the standard error of the odds ratios will not be appropriate and should be avoided.

Example 4: The (cumulative) odds ratio of **rating** $\geq j$ (for all $j = 1, \dots, J - 1$) for contact and temperature are

```
> round(exp(fm1$beta), 1)
```

```
contactyes    tempwarm
      4.6         12.2
```

attesting to the strong effects of contact and temperature. Asymmetric confidence intervals for the odds ratios based on the Wald statistic are:

```
> round(exp(confint(fm1, type = "Wald")), 1)
```

	2.5 %	97.5 %
1 2	0.1	0.7
2 3	1.5	8.2
3 4	9.9	103.4
4 5	35.7	625.8
contactyes	1.8	11.7
tempwarm	4.3	34.4

\square

Table 3: Summary of various link functions

Name	logit	probit	log-log	clog-log ^a	cauchit
Distribution	logistic	Normal	Gumbel (max) ^b	Gumbel (min) ^b	Cauchy ^c
Shape	symmetric	symmetric	right skew	left skew	kurtotic
Link function (F^{-1})	$\log[\gamma/(1-\gamma)]$	$\Phi^{-1}(\gamma)$	$-\log[-\log(\gamma)]$	$\log[-\log(1-\gamma)]$	$\tan[\pi(\gamma-0.5)]$
Inverse link (F)	$1/[1+\exp(\eta)]$	$\Phi(\eta)$	$\exp(-\exp(-\eta))$	$1-\exp[-\exp(\eta)]$	$\arctan(\eta)/\pi+0.5$
Density ($f = F'$)	$\exp(-\eta)/[1+\exp(-\eta)]^2$	$\phi(\eta)$	$\exp(-\exp(-\eta)-\eta)$	$\exp[-\exp(\eta)+\eta]$	$1/[\pi(1+\eta^2)]$

^a: the *complementary log-log* link

^b: the Gumbel distribution is also known as the extreme value (type I) distribution for extreme minima or maxima. It is also sometimes referred to as the Weibull (or log-Weibull) distribution (http://en.wikipedia.org/wiki/Gumbel_distribution).

^c: the Cauchy distribution is a *t*-distribution with one df

2.3 Link functions

Cumulative link models are not formally a member of the class of (univariate) generalized linear models⁵ (McCullagh and Nelder, 1989), but they share many similarities with generalized linear models. Notably a link function and a linear predictor ($\eta_{ij} = \theta_j - \mathbf{x}_i^T \boldsymbol{\beta}$) needs to be specified as in generalized linear models while the response distribution is just the multinomial. Fahrmeir and Tutz (2001) argues that cumulative link models are members of a class of multivariate generalized linear models. In addition to the logit link other choices are the probit, cauchit, log-log and clog-log links. These are summarized in Table 3. The cumulative link model may be written as

$$\gamma_{ij} = F(\eta_{ij}), \quad \eta_{ij} = \theta_j - \mathbf{x}_i^T \boldsymbol{\beta} \quad (4)$$

where F^{-1} is the link function—the motivation for this particular notation will be given in section 2.6.

The probit link is often used when the model is interpreted with reference to a latent variable, cf. section 2.6. When the response variable represent grouped duration or survival times the complementary log-log link is often used. This leads to the proportional hazard model for grouped responses:

$$-\log\{1 - \gamma_j(\mathbf{x}_i)\} = \exp(\theta_j - \mathbf{x}_i^T \boldsymbol{\beta})$$

or equivalently

$$\log[-\log\{1 - \gamma_j(\mathbf{x}_i)\}] = \theta_j - \mathbf{x}_i^T \boldsymbol{\beta}. \quad (5)$$

Here $1 - \gamma_j(\mathbf{x}_i)$ is the probability or survival beyond category j given \mathbf{x}_i . The proportional hazards model has the property that

$$\log\{\gamma_j(\mathbf{x}_1)\} = \exp[(\mathbf{x}_2^T - \mathbf{x}_1^T)\boldsymbol{\beta}] \log\{\gamma_j(\mathbf{x}_2)\}.$$

If the log-log link is used on the response categories in the reverse order, this is equivalent to using the c-log-log link on the response in the original order. This reverses the sign of $\boldsymbol{\beta}$ as well as the sign and order of $\{\theta_j\}$ while the likelihood and standard errors remain unchanged.

In addition to the standard links in Table 3, flexible link functions are available for `c1m` in package `ordinal`.

Table 4: Income distribution (percentages) in the Northeast US adopted from McCullagh (1980).

Year	Income						
	0-3	3-5	5-7	7-10	10-12	12-15	15+
1960	6.50	8.20	11.30	23.50	15.60	12.70	22.20
1970	4.30	6.00	7.70	13.20	10.50	16.30	42.10

Example 5: McCullagh (1980) present data on income distribution in the Northeast US reproduced in Table 4 and available in package `ordinal` as the object `income`. The unit of the income groups are thousands of (constant) 1973 US dollars. The numbers in the body of the table are percentages of the population summing to 100 in each row⁶, so these are not the original observations. The uncertainty of parameter estimates depends on the sample size, which is unknown here, so we will not consider hypothesis tests. Rather the most important systematic component is an upward shift in the income distribution from 1960 to 1970 which can be estimated from a cumulative link model. This is possible since the parameter estimates themselves only depend on the relative proportions and not the absolute numbers.

McCullagh considers which of the logit or cloglog links best fit the data in a model with an additive effect of `year`. He concludes that a the complementary log-log link corresponding to a right-skew distribution is a good choice. We can compare the relative merit of the links by comparing the value of the log-likelihood of models with different link functions:

```
> links <- c("logit", "probit", "cloglog", "loglog", "cauchit")
> sapply(links, function(link) {
  clm(income ~ year, data=income, weights=pct, link=link)$logLik })

      logit      probit    cloglog    loglog    cauchit
-353.3589 -353.8036 -352.8980 -355.6028 -353.8036
```

The `cauchit` link attains the highest log-likelihood closely followed by the complementary log-log link. This indicates that a symmetric heavy tailed distribution such as the Cauchy provides an even slightly better description of these data than a right skew distribution.

Adopting the complementary log-log link we can summarize the connection between the income in the two years by the following: If $p_{1960}(x)$ is proportion of the population with an income larger than $\$x$ in 1960 and $p_{1970}(x)$ is the equivalent in 1970, then approximately

$$\begin{aligned}\log p_{1960}(x) &= \exp(\hat{\beta}) \log p_{1970}(x) \\ &= \exp(0.568) \log p_{1970}(x)\end{aligned}\quad \square$$

2.4 Maximum likelihood estimation of cumulative link models

Cumulative link models are usually estimated by maximum likelihood (ML) and this is also the criterion used in package `ordinal`. The log-likelihood function (ignoring additive constants) can be written as

$$\ell(\boldsymbol{\theta}, \boldsymbol{\beta}; \mathbf{y}) = \sum_{i=1}^n w_i \log \pi_i \quad (6)$$

⁵the distribution of the response, the multinomial, is not a member of the (univariate) exponential family of distributions.

⁶save rounding error

where i index all scalar observations (not multinomial vector observations), w_i are potential case weights and π_i is the probability of the i th observation falling in the response category that it did, i.e., π_i are the non-zero elements of $\pi_{ij}I(Y_i = j)$. Here $I(\cdot)$ is the indicator function being 1 if its argument is true and zero otherwise. The ML estimates of the parameters; $\hat{\boldsymbol{\theta}}$ and $\hat{\boldsymbol{\beta}}$ are those values of $\boldsymbol{\theta}$ and $\boldsymbol{\beta}$ that maximize the log-likelihood function in (6).

Not all data sets can be summarized in a table like Table 1. If a continuous variable takes a unique value for each observation, each row of the resulting table would contain a single 1 and zeroes for the rest. In this case all $\{w_i\}$ are one unless the observations are weighted for some other reason. If the data can be summarized as in Table 1, a multinomial observation vector such as $[3, 1, 2]$ can be fitted using $\mathbf{y} = [1, 1, 1, 2, 3, 3]$ with $\mathbf{w} = [1, 1, 1, 1, 1, 1]$ or by using $\mathbf{y} = [1, 2, 3]$ with $\mathbf{w} = [3, 1, 2]$. The latter construction is considerably more computationally efficient (and therefore faster) since the log-likelihood function contains three rather than six terms and the design matrix, \mathbf{X} will have three rather than six rows.

The details of the actual algorithm by which the likelihood function is optimized is deferred to a later section.

According to standard likelihood theory, the variance-covariance matrix of the parameters can be obtained as the inverse of the observed Fisher information matrix. This matrix is given by the negative Hessian of the log-likelihood function⁷ evaluated at the maximum likelihood estimates. Standard errors can be obtained as the square root of the diagonal of the variance-covariance matrix.

Let $\boldsymbol{\alpha} = [\boldsymbol{\theta}, \boldsymbol{\beta}]$ denote the full set of parameters. The Hessian matrix is then given as the second order derivative of the log-likelihood function evaluated at the ML estimates:

$$\mathbf{H} = \left. \frac{\partial^2 \ell(\boldsymbol{\alpha}; \mathbf{y})}{\partial \boldsymbol{\alpha} \partial \boldsymbol{\alpha}^T} \right|_{\boldsymbol{\alpha} = \hat{\boldsymbol{\alpha}}} . \quad (7)$$

The observed Fisher information matrix is then $\mathbf{I}(\hat{\boldsymbol{\alpha}}) = -\mathbf{H}$ and the standard errors are given by

$$\text{se}(\hat{\boldsymbol{\alpha}}) = \sqrt{\text{diag}[\mathbf{I}(\hat{\boldsymbol{\alpha}})^{-1}]} = \sqrt{\text{diag}[-\mathbf{H}(\hat{\boldsymbol{\alpha}})^{-1}]} . \quad (8)$$

Another general way to obtain the variance-covariance matrix of the parameters is to use the expected Fisher information matrix. The choice of whether to use the observed or the expected Fisher information matrix is often dictated by the fitting algorithm: re-weighted least squares methods often produce the expected Fisher information matrix as a by-product of the algorithm, and Newton-Raphson algorithms (such as the one used for `c1m` in `ordinal`) similarly produce the observed Fisher information matrix. Efron and Hinkley (1978) considered the choice of observed versus expected Fisher information and argued that the observed information contains relevant information thus it is preferred over the expected information.

Pratt (1981) and Burridge (1981) showed (seemingly independent of each other) that the log-likelihood function of cumulative link models with the link functions considered in Table 3, except for the cauchit link, is concave. This means that there is a unique global optimum so there is no risk of convergence to a local optimum. It also means that the step of a Newton-Raphson algorithm is guaranteed to be in the direction of a higher likelihood although the step may be too large to cause an increase in the likelihood. Successively halving the step whenever this happens effectively ensures convergence.

⁷equivalently the Hessian of the negative log-likelihood function.

Notably the log likelihood of cumulative cauchit models is not guarantied to be concave, so convergence problems may occur with the Newton-Raphson algorithm. Using the estimates from a cumulative probit models as starting values seems to be a widely successful approach.

Observe also that the concavity property does not extend to cumulative link models with scale effects, but that structured thresholds (cf. section 2.7) are included.

2.5 Deviance and model comparison

2.5.1 Model comparison with likelihood ratio tests

A general way to compare models is by means of the likelihood ratio statistic. Consider two models, m_0 and m_1 , where m_0 is a submodel of model m_1 , that is, m_0 is simpler than m_1 and m_0 is *nested* in m_1 . The likelihood ratio statistic for the comparison of m_0 and m_1 is

$$LR = -2(\ell_0 - \ell_1) \quad (9)$$

where ℓ_0 is the log-likelihood of m_0 and ℓ_1 is the log-likelihood of m_1 . The likelihood ratio statistic measures the evidence in the data for the extra complexity in m_1 relative to m_0 . The likelihood ratio statistic asymptotically follows a χ^2 distribution with degrees of freedom equal to the difference in the number of parameter of m_0 and m_1 . The likelihood ratio test is generally more accurate than Wald tests. Cumulative link models can be compared by means of likelihood ratio tests with the `anova` method.

Example 6: Consider the additive model for the wine data in example 3 with a main effect of temperature and contact. We can use the likelihood ratio test to assess whether the interaction between these factors are supported by the data:

```
> fm2 <- clm(rating ~ contact * temp, data = wine)
> anova(fm1, fm2)
```

Likelihood ratio tests of cumulative link models:

	formula:	link:	threshold:
fm1	rating ~ contact + temp	logit	flexible
fm2	rating ~ contact * temp	logit	flexible

	no.par	AIC	logLik	LR.stat	df	Pr(>Chisq)
fm1	6	184.98	-86.492			
fm2	7	186.83	-86.416	0.1514	1	0.6972

The likelihood ratio statistic is small in this case and compared to a χ^2 distribution with 1 df, the p -value turns out insignificant. We conclude that the interaction is not supported by the data. \square

2.5.2 Deviance and ANODE tables

In linear models ANOVA tables and F -tests are based on the decomposition of sums of squares. The concept of sums of squares does not make much sense for categorical observations, but a more general measure called the *deviance* is defined for generalized linear models and contingency tables⁸. The deviance can be used in much the same way to compare nested

⁸i.e., for likelihood based models for contingency tables

models and to make a so-called analysis of deviance (ANODE) table. The deviance is closely related to sums of squares for linear models (McCullagh and Nelder, 1989).

The deviance is defined as minus twice the difference between the log-likelihoods of a *full* (or *saturated*) model and a reduced model:

$$D = -2(\ell_{\text{reduced}} - \ell_{\text{full}}) \quad (10)$$

The full model has a parameter for each observation and describes the data perfectly while the reduced model provides a more concise description of the data with fewer parameters.

A special reduced model is the *null model* which describes no other structure in the data than what is implied by the design. The corresponding deviance is known as the *null deviance* and analogous to the total sums of squares for linear models. The null deviance is therefore also denoted the *total deviance*. The *residual deviance* is a concept similar to a residual sums of squares and simply defined as

$$D_{\text{resid}} = D_{\text{total}} - D_{\text{reduced}} \quad (11)$$

A *difference in deviance* between two nested models is identical to the likelihood ratio statistic for the comparison of these models. Thus the deviance difference, just like the likelihood ratio statistic, asymptotically follows a χ^2 -distribution with degrees of freedom equal to the difference in the number of parameters in the two models. In fact the deviance in (10) is just the likelihood ratio statistic for the comparison of the full and reduced models.

The likelihood of reduced models are available from fits of cumulative link models, but since it is not always easy to express the full model as a cumulative link model, the log-likelihood of the full model has to be obtained in another way. For a two-way table like Table 1 indexed by h (rows) and j (columns), the log-likelihood of the full model (comparable to the likelihood in (6)) is given by

$$\ell_{\text{full}} = \sum_h \sum_j w_{hj} \log \hat{\pi}_{hj} \quad (12)$$

where $\hat{\pi}_{hj} = w_{hj}/w_{h\cdot}$, w_{hj} is the count in the (h, j) th cell and $w_{h\cdot}$ is the sum in row h .

Example 7: We can get the likelihood of the full model for the wine data in Table 1 with

```
> tab <- with(wine, table(temp:contact, rating))
> ## Get full log-likelihood:
> pi.hat <- tab / rowSums(tab)
> (ll.full <- sum(tab * ifelse(pi.hat > 0, log(pi.hat), 0))) ## -84.01558

[1] -84.01558
```

The total deviance (10) for the wine data is given by

```
> ## fit null-model:
> fm0 <- clm(rating ~ 1, data = wine)
> ll.null <- fm0$logLik
> ## The null or total deviance:
> (Deviance <- -2 * (ll.null - ll.full)) ## 39.407

[1] 39.407
```

□

Example 8: An ANODE table for the wine data in Table 1 is presented in Table 5 where the total deviance is broken up into model deviance (due to treatments) and residual deviance.

Table 5: ANODE table for the data in Table 1.

Source	df	deviance	<i>p</i> -value
Total	12	39.407	< 0.001
Treatment	3	34.606	< 0.001
Temperature, <i>T</i>	1	26.928	< 0.001
Contact, <i>C</i>	1	11.043	< 0.001
Interaction, <i>T</i> × <i>C</i>	1	0.1514	0.6972
Residual	9	4.8012	0.8513

Further, the treatment deviance is described by contributions from main effects and interaction. Observe that the deviances for the main effects and interaction do not add up to the deviance for Treatment as the corresponding sums of squares would have in a analogous linear model (ANOVA)⁹. The deviances for these terms can instead be interpreted as likelihood ratio tests of nested models: the deviance for the interaction term is the likelihood ratio statistics of the interaction controlling for the main effects, and the deviances for the main effects are the likelihood ratio statistics for these terms while controlling for the other main effect and ignoring the interaction term. As is clear from Table 5, there are significant treatment differences and these seem to describe the data well since the residual deviance is insignificant—the latter is a goodness of fit test for the cumulative logit model describing treatment differences. Further, the treatment differences are well captured by the main effects and there is no indication of an important interaction. □

The terminology can be a bit confusing in this area. Sometimes any difference in deviance between two nested models, i.e., a likelihood ratio statistic is denoted a deviance and sometimes any quantity that is proportional to minus twice the log-likelihood of a model is denoted the deviance of that model.

2.5.3 Goodness of fit tests with the deviance

The deviance can be used to test the goodness of fit of a particular reduced model. The deviance asymptotically follows as χ^2 distribution with degrees of freedom equal to the difference in the number of parameters between the two models. The asymptotics are generally good if the expected frequencies under the reduced model are not too small and as a general rule they should all be at least five. This provides a goodness of fit test of the reduced model. The expectation of a random variable that follows a χ^2 -distribution is equal to the degrees of freedom of the distribution, so as a rule of thumb, if the deviance in (10) is about the same size as the difference in the number of parameters, there is not evidence of lack of fit.

One problem with the deviance for a particular (reduced) model is that it depends on which model is considered the full model, i.e., how the total deviance is calculated, which often derives from the tabulation of the data. Observe that differences in deviance for nested models are independent of the likelihood of a full model, so deviance differences are insensitive to this choice. Collett (2002) recommends that the data are aggregated as much as possible when evaluating deviances and goodness of fit tests are performed.

Example 9: In the presentation of the wine data in example 1 and Table 1, the data were aggregated over judges and bottles. Had we included `bottle` in the tabulation of the data we

⁹This holds for orthogonal designs including balanced and complete tables like Table 1.

Table 6: Table of the wine data similar to Table 1, but including bottle in the tabulation.

Temperature	Contact	Bottle	Least—Most bitter				
			1	2	3	4	5
cold	no	1	3	4	2	0	0
cold	no	2	1	5	3	0	0
cold	yes	3	1	2	5	1	0
cold	yes	4	0	5	3	1	0
warm	no	5	0	3	4	1	1
warm	no	6	0	2	4	2	1
warm	yes	7	0	1	2	2	4
warm	yes	8	0	0	3	5	1

would have arrived at Table 6. A full model for the data in Table 1 has $(5 - 1)(4 - 1) = 12$ degrees of freedom while a full model for Table 6 has $(5 - 1)(8 - 1) = 28$ degrees of freedom and a different deviance.

If it is decided that bottle is not an important variable, Collett's recommendation is that we base the residual deviance on a full model defined from Table 1 rather than Table 6. \square

2.6 Latent variable motivation for cumulative link models

A cumulative link model can be motivated by assuming an underlying continuous latent variable, S with cumulative distribution function, F . The ordinal response variable, Y_i is then observed in category j if S_i is between the thresholds $\theta_{j-1}^* < S_i \leq \theta_j^*$ where

$$-\infty \equiv \theta_0^* < \theta_1^* < \dots < \theta_{J-1}^* < \theta_J^* \equiv \infty$$

divide the real line on which S lives into $J + 1$ intervals. The situation is illustrated in Fig. 2 where a probit link and $J = 4$ is adopted. The three thresholds, $\theta_1, \theta_2, \theta_3$ divide the area under the curve into four parts each of which represent the probability of a response falling in the four response categories. The thresholds are fixed on the scale, but the location of the latent distribution, and therefore also the four areas under the curve, changes with \mathbf{x}_i . A normal linear model for the latent variable is

$$S_i = \alpha + \mathbf{x}_i^T \boldsymbol{\beta}^* + \varepsilon_i, \quad \varepsilon_i \sim N(0, \sigma^2) \quad (13)$$

where $\{\varepsilon_i\}$ are random disturbances and α is the intercept, i.e., the mean value of S_i when \mathbf{x}_i correspond to a reference level for factors and to zero for continuous covariates. Equivalently we could write: $S_i \sim N(\alpha + \mathbf{x}_i^T \boldsymbol{\beta}^*, \sigma^2)$.

The cumulative probability of an observation falling in category j or below is then:

$$\gamma_{ij} = P(Y_i \leq j) = P(S_i \leq \theta_j^*) = P\left(Z_i \leq \frac{\theta_j^* - \alpha - \mathbf{x}_i^T \boldsymbol{\beta}^*}{\sigma}\right) = \Phi\left(\frac{\theta_j^* - \alpha - \mathbf{x}_i^T \boldsymbol{\beta}^*}{\sigma}\right) \quad (14)$$

where $Z_i = (S_i - \alpha - \mathbf{x}_i^T \boldsymbol{\beta}^*)/\sigma \sim N(0, 1)$ and Φ is the standard normal CDF.

Since the absolute location and scale of the latent variable, α and σ respectively, are not identifiable from ordinal observations, an identifiable model is

$$\gamma_{ij} = \Phi(\theta_j - \mathbf{x}_i^T \boldsymbol{\beta}), \quad (15)$$

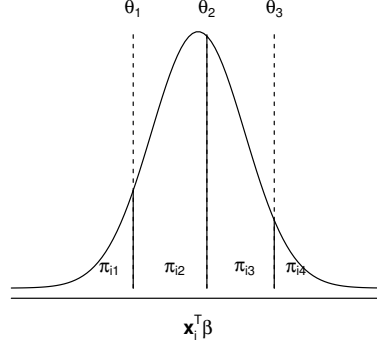


Figure 2: Illustration of a cumulative link model in terms of the latent distribution.

with identifiable parameter functions:

$$\theta_j = (\theta_j^* - \alpha)/\sigma \quad \text{and} \quad \beta = \beta^*/\sigma . \quad (16)$$

Observe how the minus in (15) entered naturally such that a positive β means a shift of the latent distribution in a positive direction.

Model (15) is exactly a cumulative link model with a probit link. Other distributional assumptions for S correspond to other link functions. In general assuming that the cumulative distribution function of S is F corresponds to assuming the link function is F^{-1} , cf. Table 3.

Some expositions of the latent variable motivation for cumulative link models get around the identifiability problem by introducing restrictions on α and σ , usually $\alpha = 0$ and $\sigma = 1$ are chosen, which leads to the same definition of the threshold and regression parameters that we use here. However, it seems misleading to introduce restrictions on unidentifiable parameters. If observations really arise from a continuous latent variable, α and σ are real unknown parameters and it makes little sense to restrict them to take certain values. This draws focus from the appropriate *relative* signal-to-ratio interpretation of the parameters evident from (16).

The standard form of the logistic distribution has mean zero and variance $\pi^2/3$. The logistic distribution is symmetric and shows a some resemblance with a normal distribution with the same mean and variance in the central part of the distribution; the tails of the logistic distribution are a little heavier than the tails of the normal distribution. In Fig. 3 the normal and logistic distributions are compared with variance $\pi^2/3$. Therefore, to a reasonable approximation, the parameters of logit and probit models are related in the following way:

$$\theta_j^{\text{probit}} \approx \theta_j^{\text{logit}}/(\pi/\sqrt{3}) \quad \text{and} \quad \beta^{\text{probit}} \approx \beta^{\text{logit}}/(\pi/\sqrt{3}) , \quad (17)$$

where $\pi/\sqrt{3} \approx 1.81$

Example 10: Considering once again the wine data the coefficients from logit and probit models with additive effects of temperature and contact are

```
> fm1 <- clm(rating ~ contact + temp, data = wine, link = "logit")
> fm2 <- clm(rating ~ contact + temp, data = wine, link = "probit")
> structure(rbind(coef(fm1), coef(fm2)),
            dimnames=list(c("logit", "probit"), names(coef(fm1))))
```

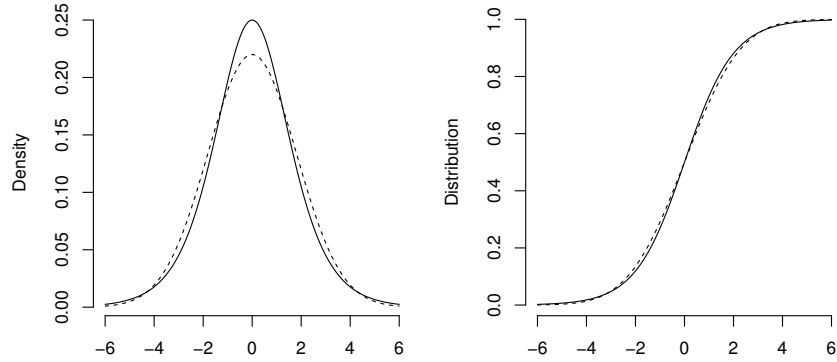



Figure 3: Left: densities. Right: distributions of logistic (solid) and normal (dashed) distributions with mean zero and variance $\pi^2/3$ which corresponds to the standard form for the logistic distribution.

	1 2	2 3	3 4	4 5	contactyes	tempwarm
logit	-1.3443834	1.2508088	3.466887	5.006404	1.5277977	2.503102
probit	-0.7732627	0.7360215	2.044680	2.941345	0.8677435	1.499375

In comparison the approximate probit estimates using (17) are

```
> coef(fm1) / (pi / sqrt(3))
```

	1 2	2 3	3 4	4 5	contactyes	tempwarm
	-0.7411974	0.6896070	1.9113949	2.7601753	0.8423190	1.3800325

These estimates are a great deal closer to the real probit estimates than the unscaled logit estimates. The average difference between the probit and approximate probit estimates being -0.079. \square

2.6.1 More on parameter interpretation

Observe that the regression parameter in cumulative link models, cf. (16) are signal-to-noise ratios. This means that adding a covariate to a cumulative link model that reduces the residual noise in the corresponding latent model will increase the signal-to-noise ratios. Thus adding a covariate will (often) increase the coefficients of the other covariates in the cumulative link model. This is different from linear models, where (in orthogonal designs) adding a covariate does not alter the value of the other coefficients¹⁰. Bauer (2009), extending work by Winship and Mare (1984) suggests a way to rescale the coefficients such they are comparable in size during model development. See also Fielding (2004).

Example 11: Consider the estimate of `temp` in models for the wine data ignoring and controlling for `contact`, respectively:

```
> coef(clm(rating ~ temp, data = wine, link = "probit"))["tempwarm"]

tempwarm
1.37229
```

¹⁰but the same thing happens in other generalized linear models, e.g., binomial and Poisson models, where the variance is determined by the mean.

```
> coef(clm(rating ~ temp + contact, data = wine, link = "probit"))["tempwarm"]
```

```
tempwarm
1.499375
```

and observe that the estimate of `temp` is larger when controlling for `contact`. In comparison the equivalent estimates in linear models are not affected—here we use the observed scores for illustration:

```
> coef(lm(as.numeric(rating) ~ temp, data = wine))["tempwarm"]
```

```
tempwarm
1.166667
```

```
> coef(lm(as.numeric(rating) ~ contact + temp, data = wine))["tempwarm"]
```

```
tempwarm
1.166667
```

In this case the coefficients are exactly identical, but in designs that are not orthogonal and observed studies with correlated covariates they will only be approximately the same. \square

Regardless of how the threshold parameters discretize the scale of the latent variable, the regression parameters β have the same interpretation. Thus β have the same meaning whether the ordinal variable is measured in, say, five or six categories. Further, the nature of the model interpretation will not change if two or more categories are amalgamated, while parameter estimates will, of course, not be completely identical. This means that regression parameter estimates can be compared (to the extent that the noise level is the same) across studies where response scales with a different number of response categories are adopted. In comparison, for linear models used on scores, it is not so simple to just combine two scores, and parameter estimates from different linear models are not directly comparable.

If the latent variable, S_i is approximated by scores assigned to the response variable, denote this variable Y_i^* , then a linear model for Y_i^* can provide approximate estimates of β by applying (16) for cumulative probit models¹¹. The quality of the estimates rest on a number of aspects:

- The scores assigned to the ordinal response variable should be structurally equivalent to the thresholds, θ^* that generate Y_i from S_i . In particular, if the (equidistant) numbers $1, \dots, J$ are the scores assigned to the response categories, the thresholds, θ^* are also assumed to be equidistant.
- The distribution of Y_i^* should not deviate too much from a bell-shaped curve; especially there should not be too many observations in the end categories
- By appeal to the central limit theorem the coarsening of S_i into Y_i^* will “average out” such that bias due to coarsening is probably small.

This approximate estimation scheme extends to other latent variable distributions than the normal where linear models are exchanged with the appropriate location-scale models, cf. Table 3.

¹¹these approximate regression parameters could be used as starting values for an iterative algorithm to find the ML estimates of β , but we have not found it worth the trouble in our Newton algorithm

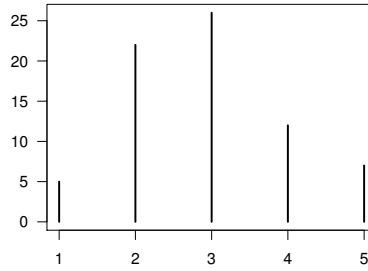


Figure 4: Histogram of the ratings in the wine data, cf. Table 1.

Example 12: Consider the following linear model for the rating scores of the wine data, cf. Table 1:

$$Y_i^* = \alpha + \beta_1 \text{temp}_i + \beta_2 \text{contact}_i + \varepsilon_i \quad \varepsilon_i \sim N(0, \sigma_\varepsilon^2)$$

The relative parameter estimates, $\tilde{\beta}$ are

```
> lm1 <- lm(as.numeric(rating) ~ contact + temp, data = wine)
> sd.lm1 <- summary(lm1)$sigma
> coef(lm1)[-1] / sd.lm1
```

```
contactyes    tempwarm
  0.791107     1.384437
```

which should be compared with the estimates from the corresponding cumulative probit model:

```
> fm1 <- clm(rating ~ contact + temp, data = wine, link = "probit")
> coef(fm1)[-1:4]
```

```
contactyes    tempwarm
  0.8677435    1.4993746
```

The relative estimates from the linear model are a lower than the cumulative probit estimates, which is a consequence of the fact that the assumptions for the linear model are not fulfilled. In particular the distance between the thresholds is not equidistant:

```
> diff(coef(fm1)[1:4])

      2|3      3|4      4|5
1.5092842 1.3086590 0.8966645
```

while the distribution is probably sufficiently bell-shaped, cf. Fig 4.

□

2.7 Structured thresholds

In this section we will motivate and describe structures on the thresholds in cumulative link models. Three options are available in `clm` using the `threshold` argument: `flexible`, `symmetric` and `equidistant` thresholds. The default option is `"flexible"`, which corresponds to the conventional ordered, but otherwise unstructured thresholds. The `"symmetric"` option restricts the thresholds to be symmetric while the `"equidistant"` option restricts the thresholds to be equally spaced.

Table 7: Symmetric thresholds with six response categories use the three parameters a , b and c .

θ_1	θ_2	θ_3	θ_4	θ_5
$-b + c$	$-a + c$	c	$a + c$	$b + c$

Table 8: Symmetric thresholds with seven response categories use the four parameters, a , b , c and d .

θ_1	θ_2	θ_3	θ_4	θ_5	θ_6
$-b + c$	$-a + c$	c	d	$a + d$	$b + d$

2.7.1 Symmetric thresholds

The basic cumulative link model assumed that the thresholds are constant for all values of $\mathbf{x}_i^T \boldsymbol{\beta}$, that they are ordered and finite but otherwise without structure. In questionnaire type response scales, the question is often of the form “how much do you agree with *statement*” with response categories ranging from “completely agree” to “completely disagree” in addition to a number of intermediate categories possibly with appropriate anchoring words. In this situation the response scale is meant to be perceived as being symmetric, thus, for example, the end categories are equally far from the central category/categories. Thus, in the analysis of such data it can be relevant to restrict the thresholds to be symmetric or at least test the hypothesis of symmetric thresholds against the more general alternative requiring only that the thresholds are ordered in the conventional cumulative link model. An example with six response categories and five thresholds is given in Table 7 where the central threshold, θ_3 maps to c while a and b are *spacings* determining the distance to the remaining thresholds. Symmetric thresholds is a parsimonious alternative since three rather than five parameters are required to determine the thresholds in this case. Naturally at least four response categories, i.e., three thresholds are required for the symmetric thresholds to use less parameters than the general alternative. With an even number of thresholds, we use a parameterization with two central thresholds as shown in Table 8.

Example 13: I am missing some good data to use here. □

2.7.2 Equidistant thresholds

Ordinal data sometimes arise when the intensity of some perception is rated on an ordinal response scale. An example of such a scale is the ratings of the bitterness of wine described in example 1. In such cases it is natural to hypothesize that the thresholds are equally spaced, or equidistant as we shall denote this structure. Equidistant thresholds use only two parameters and our parameterization can be described by the following mapping:

$$\theta_j = a + b(j - 1), \quad \text{for } j = 1, \dots, J - 1 \quad (18)$$

such that $\theta_1 = a$ is the first threshold and b denotes the distance between adjacent thresholds.

Example 14: In example 3 we fitted a model for the wine data (cf. Table 1) with additive effects of temperature and contact while only restricting the thresholds to be suitably ordered. For convenience this model fit is repeated here:

```
> fm1 <- clm(rating ~ temp + contact, data=wine)
> summary(fm1)
```

```

formula: rating ~ temp + contact
data:    wine

link threshold nobs logLik AIC      niter max.grad cond.H
logit flexible 72   -86.49 184.98 6(0)  4.02e-12 2.7e+01

Coefficients:
              Estimate Std. Error z value Pr(>|z|)
tempwarm      2.5031      0.5287   4.735 2.19e-06 ***
contactyes     1.5278      0.4766   3.205 0.00135 **
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

```

```

Threshold coefficients:
              Estimate Std. Error z value
1|2  -1.3444      0.5171  -2.600
2|3   1.2508      0.4379   2.857
3|4   3.4669      0.5978   5.800
4|5   5.0064      0.7309   6.850

```

The successive distances between the thresholds in this model are

```

> diff(fm1$alpha)

      2|3      3|4      4|5
2.595192 2.216078 1.539517

```

so the distance between the thresholds seems to be decreasing. However, the standard errors of the thresholds are about half the size of the distances, so their position is not that well determined. A model where the thresholds are restricted to be equally spaced is fitted with

```

> fm2 <- clm(rating ~ temp + contact, data=wine, threshold="equidistant")
> summary(fm2)

```

```

formula: rating ~ temp + contact
data:    wine

link threshold  nobs logLik AIC      niter max.grad cond.H
logit equidistant 72   -87.86 183.73 5(0)  4.80e-07 3.2e+01

```

```

Coefficients:
              Estimate Std. Error z value Pr(>|z|)
tempwarm      2.4632      0.5164   4.77 1.84e-06 ***
contactyes     1.5080      0.4712   3.20 0.00137 **
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

```

```

Threshold coefficients:
              Estimate Std. Error z value
threshold.1 -1.0010      0.3978  -2.517
spacing      2.1229      0.2455   8.646

```

so here $\hat{\theta}_1 = \hat{a} = -1.001$ and $\hat{b} = 2.123$ in the parameterization of (18). We can test the assumption of equidistant thresholds against the flexible alternative with a likelihood ratio test:

```

> anova(fm1, fm2)

```

Likelihood ratio tests of cumulative link models:

```

      formula:                      link: threshold:
fm2 rating ~ temp + contact logit equidistant
fm1 rating ~ temp + contact logit flexible

      no.par    AIC  logLik LR.stat df Pr(>Chisq)
fm2      4 183.73 -87.865
fm1      6 184.98 -86.492  2.7454  2      0.2534

```

so the p -value is $p = 0.253$ not providing much evidence against equidistant thresholds. \square

3 Assessing the likelihood and model convergence

Cumulative link models are non-linear models and in general the likelihood function of non-linear models is not guaranteed to be well behaved or even uni-modal. However, as mentioned in section 2.4 Pratt (1981) and Burrige (1981) showed that the log-likelihood function of cumulative link models with the link functions considered in Table 3, except for the cauchit link, is concave. This means that there is a unique global optimum so there is no risk of convergence to a local optimum. There is no such guarantee in more general models.

There are no closed form expressions for the ML estimates of the parameters in cumulative link models. This means that iterative methods have to be used to fit the models. There is no guarantee that the iterative method converges to the optimum. In complicated models the iterative method may terminate at a local optimum or just far from the optimum resulting in inaccurate parameter estimates. We may hope that the optimization process warns about non-convergence, but that can also fail. To be sure the likelihood function is well behaved and that an unequivocal optimum has been reached we have to inspect the likelihood function in a neighborhood around the optimum as reported by the optimization.

As special feature for cumulative link models, the threshold parameters are restricted to be ordered and therefore naturally bounded. This may cause the log-likelihood function to be irregular for one or more parameters. This also motivates visualizing the likelihood function in the neighborhood of the optimum. To do this we use the `slice` function. As the name implies, it extracts a (one-dimensional) slice of the likelihood function.

We use the likelihood slices for two purposes:

1. To visualize and inspect the likelihood function in a neighborhood around the optimum. We choose a rather large neighborhood and look at how well-behaved the likelihood function is, how close to a quadratic function it is, and if there is only one optimum.
2. To verify that the optimization converged and that the parameter estimates are accurately determined. For this we choose a rather narrow neighborhood around the optimum.

The log-likelihood slice is defined as

$$\ell_{\text{slice}}(\alpha_a; \mathbf{y}) = \ell(\alpha_a, \hat{\alpha}_{-a}; \mathbf{y}) , \quad (19)$$

where $\boldsymbol{\alpha}$ denotes the joint parameter vector. Thus the slice is the log-likelihood function regarded as a function of the a th parameter while the remaining parameters are fixed at their ML estimates.

The Hessian at the optimum measures the curvature in the log-likelihood function in the parameter space. To scale the range of the parameters at which the likelihood is sliced, we consider the following measures of curvature:

$$\boldsymbol{\zeta} = \sqrt{\text{diag}(-\mathbf{H})} \quad (20)$$

Here $\boldsymbol{\zeta}$ is a $(q + p)$ -vector of curvature units for the q threshold parameters $\boldsymbol{\theta}$ and the p regression parameters $\boldsymbol{\beta}$. We can understand $\boldsymbol{\zeta}$ as a vector of standard errors which are not controlled for the dependency of the other parameters. Indeed, if the parameters are completely uncorrelated, \mathbf{H} is diagonal and $\boldsymbol{\zeta}$ coincide with standard errors, cf. (8), however, this is not possible in cumulative link models.

The range of the parameters at which the log-likelihood is sliced is then a simple multiple (λ) of the curvature units in each direction: $\lambda\boldsymbol{\zeta}$. Working in curvature units is a way to standardize the parameter range even if some parameters are much better determined (much less curvature in the log-likelihood) than others.

A well-behave log-likelihood function will be approximately quadratic in shape in a neighborhood around the optimum. Close enough to the optimum, the log-likelihood function will be virtually indistinguishable from a quadratic approximation if all parameters are identified. For the a th parameter the quadratic approximation to the log-likelihood function is given by

$$-\frac{(\hat{\alpha}_a - \alpha_a)^2}{2\zeta_a^2}.$$

Example 15: Consider again a cumulative link model for the wine data. In the following we ask for a slice of the log-likelihood function for each of the parameters and plot these. By setting $\lambda = 5$ we ask for the slice in a rather wide neighborhood around the optimum:

```
> fm1 <- clm(rating ~ temp + contact, data=wine)
> slice.fm1 <- slice(fm1, lambda = 5)
> par(mfrow = c(2, 3))
> plot(slice.fm1)
```

The result is shown in Fig. 5. By default the quadratic approximation is included for reference in the plot.

For this model we see that the log-likelihood function is nicely quadratic for the regression parameters while it is less so for the threshold parameters and particularly bad for the end thresholds. The log-likelihood is *relative* as indicated by the label on the vertical axis since the values are relative to the maximum log-likelihood value.

From Fig. 5 it seems that the parameter estimates as indicated by the vertical bars are close to the optimum indicating successful model convergence. To investigate more closely we slice the likelihood at a much smaller scale using $\lambda = 10^{-5}$:

```
> slice2.fm1 <- slice(fm1, lambda = 1e-5)
> par(mfrow = c(2, 3))
> plot(slice2.fm1)
```

The resulting figure is shown in Fig. 6. Observe that 1) the model has converged, 2) from inspection of the horizontal axis all parameters estimates are correct to at least six decimals, 3) the quadratic approximation is indistinguishable from the log-likelihood at this scale and 4) from the vertical axis the log-likelihood value is determined accurately to at least 12 digits. \square

Example 16: Example with confidence contours. \square

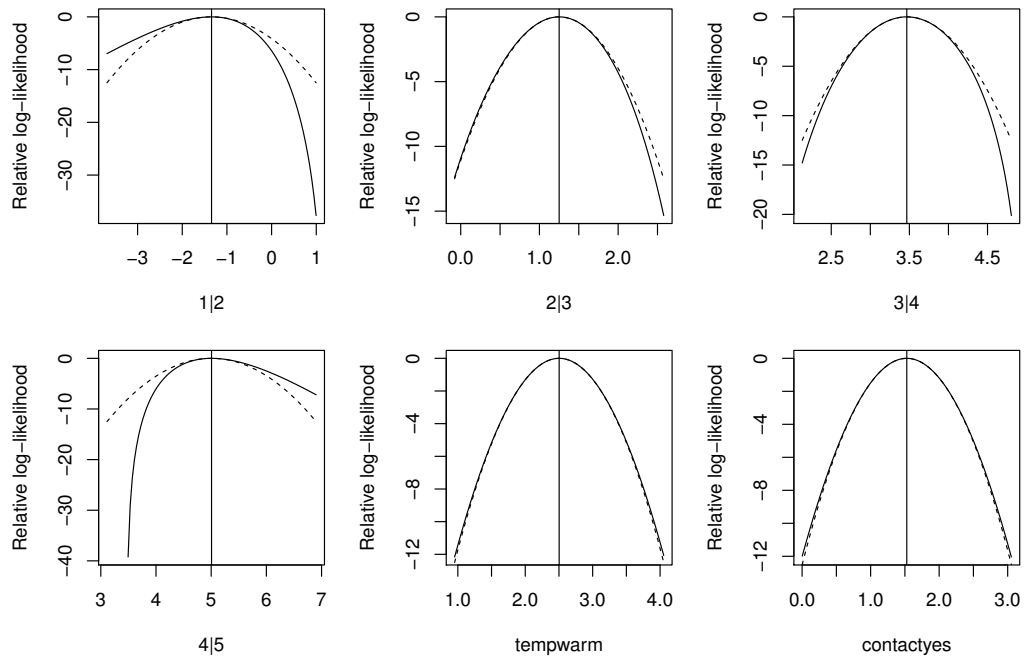


Figure 5: Slices of the log-likelihood function for parameters in a model for the bitterness-of-wine data. Dashed lines indicate quadratic approximations to the log-likelihood function and vertical bars indicate maximum likelihood estimates.

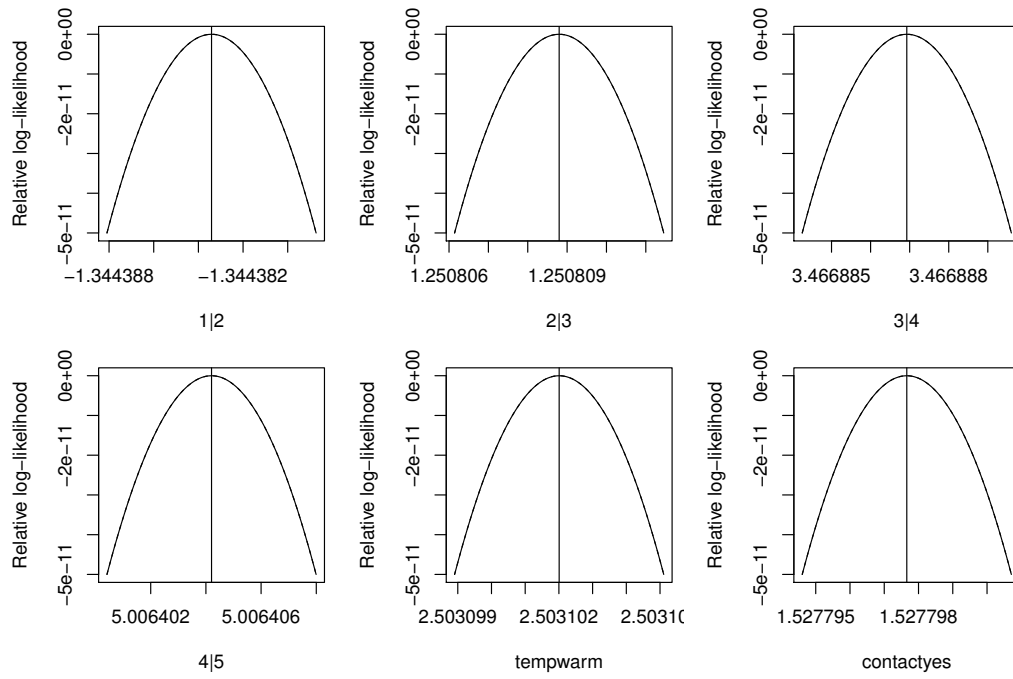


Figure 6: Slices of the log-likelihood function for parameters in a model for the bitterness-of-wine data very close to the MLEs. Dashed lines indicate quadratic approximations to the log-likelihood function and vertical bars the indicate maximum likelihood estimates.

Unfortunately there is no general way to infer confidence intervals from the likelihood slices—for that we have to use the computationally more intensive profile likelihoods. Compared to the profile likelihoods discussed in section 4, the slice is much less computationally demanding since the likelihood function is only evaluated—not optimized, at a range of parameter values.

4 Confidence intervals and profile likelihood

Confidence intervals are convenient for summarizing the uncertainty about estimated parameters. The classical symmetric estimates given by $\hat{\beta} \pm z_{1-\alpha/2} \text{se}(\hat{\beta})$ are based on the Wald statistic¹², $w(\beta) = (\hat{\beta} - \beta) / \text{se}(\hat{\beta})$ and available by `confint(fm1, type = "Wald")`. A similar result could be obtained by `confint.default(fm1)`. However, outside linear models asymmetric confidence intervals often better reflect the uncertainty in the parameter estimates. More accurate, and generally asymmetric, confidence intervals can be obtained by using the likelihood root statistic instead; this relies on the so-called profile likelihood written here for an arbitrary scalar parameter β_a :

$$\ell_p(\beta_a; \mathbf{y}) = \max_{\boldsymbol{\theta}, \boldsymbol{\beta}_{-a}} \ell(\boldsymbol{\theta}, \boldsymbol{\beta}; \mathbf{y}) ,$$

where $\boldsymbol{\beta}_{-a}$ is the vector of regression parameters without the a th one. In words, the profile log-likelihood for β_a is given as the full log-likelihood optimized over all parameters but β_a . To obtain a smooth function, the likelihood is optimized over a range of values of β_a around the ML estimate, $\hat{\beta}_a$, further, these points are interpolated by a spline to provide an even smoother function.

The likelihood root statistic (see e.g., Pawitan, 2001; Brazzale et al., 2007) is defined as:

$$r(\beta_a) = \text{sign}(\hat{\beta}_a - \beta_a) \sqrt{-2[\ell(\hat{\boldsymbol{\theta}}, \hat{\boldsymbol{\beta}}; \mathbf{y}) - \ell_p(\beta_a; \mathbf{y})]}$$

and just like the Wald statistic its reference distribution is the standard normal. Confidence intervals based on the likelihood root statistic are defined as those values of β_a for which $r(\beta_a)$ is in between specified bounds, e.g., -1.96 and 1.96 for 95% confidence intervals. Formally the confidence intervals are defined as

$$CI : \{ \beta_a; |r(\beta_a)| < z_{1-\alpha/2} \} .$$

Example 17: Consider again a model for the wine data. The profile likelihood confidence intervals are obtained with

```
> fm1 <- glm(rating ~ temp + contact, data=wine)
> confint(fm1)
```

```

          2.5 %    97.5 %
tempwarm  1.5097627 3.595225
contactyes 0.6157925 2.492404
```

where we would have appended `type = "profile"` since this is the default. Confidence intervals with other confidence levels are obtained using the `level` argument. The equivalent confidence intervals based on the Wald statistic are

```
> confint(fm1, type = "Wald")
```

¹²where $z_{1-\alpha/2}$ is the $(1 - \alpha/2)$ -quantile of the standard normal CDF.

	2.5 %	97.5 %
1 2	-2.3578848	-0.330882
2 3	0.3925794	2.109038
3 4	2.2952980	4.638476
4 5	3.5738541	6.438954
tempwarm	1.4669081	3.539296
contactyes	0.5936345	2.461961

In this case the Wald bounds are a little too low compared to the profile likelihood confidence bounds. \square

Visualization of the likelihood root statistic can be helpful in diagnosing non-linearity in the parameterization of the model. The linear scale is particularly suited for this rather than other scales, such as the quadratic scale at which the log-likelihood lives.

The `plot` method for `profile` objects that can produce a range of different plots on different scales. The `plot` method takes the following arguments:

```
function (x, which.par = seq_len(nprofiles), level = c(0.95, 0.99),
  Log = FALSE, relative = TRUE, root = FALSE, fig = TRUE, approx = root,
  n = 1000, ask = prod(par("mfcol")) < length(which.par) && dev.interactive(),
  ..., ylim = NULL)
```

If `root = TRUE` an approximately linear plot of β_a versus $-r(\beta_a)$ is produced¹³. If `approx = TRUE` (the default when `root = TRUE`) the Wald statistic is also included on the square root scale, $-\sqrt{w(\beta_a)}$. This is the tangent line to $-r(\beta_a)$ at $\hat{\beta}_a$ and provides a reference against which to measure curvature in $r(\beta_a)$. Horizontal lines at ± 1.96 and ± 2.58 indicate 95% and 99% confidence intervals.

When `root = FALSE`, the `Log` argument controls whether the likelihood should be plotted on the log scale, and similarly the `relative` argument controls whether the absolute or relative (log-) likelihood should be plotted. At the default settings, the `plot` method produce a plot

Example 18: Consider the model from the previous example. The likelihood root statistic can be obtained with

```
> pr1 <- profile(fm1, which.beta="tempwarm")
> plot(pr1, root=TRUE)
```

The resulting figure is shown in Fig. 7. A slight skewness in the profile likelihood for `tempwarm` translates into curvature in the likelihood root statistic. The Wald and profile likelihood confidence intervals are given as intersections with the horizontal lines. \square

In summarizing the results of a models fit, I find the relative likelihood scale, $\exp(-r(\beta_a)^2/2) = \exp\{\ell(\hat{\theta}, \hat{\beta}; \mathbf{y}) - \ell_p(\beta_a; \mathbf{y})\}$ informative. The evidence about the parameters is directly visible on this scale (cf. Fig. 8); the ML estimate has maximum support, and values away from here are less supported by the data, 95% and 99% confidence intervals are readily read of the plots as intersections with the horizontal lines. Most importantly the plots emphasize that a range of parameter values are actually quite well supported by the data—something which is easy to forget when focus is on the exact numbers representing the ML estimates.

Example 19: The relative profile likelihoods are obtained with

```
> pr1 <- profile(fm1, alpha=1e-4)
> plot(pr1)
```

¹³actually we reversed the sign of the statistic in the display since a line from lower-left to upper-right looks better than a line from upper-left to lower-right.

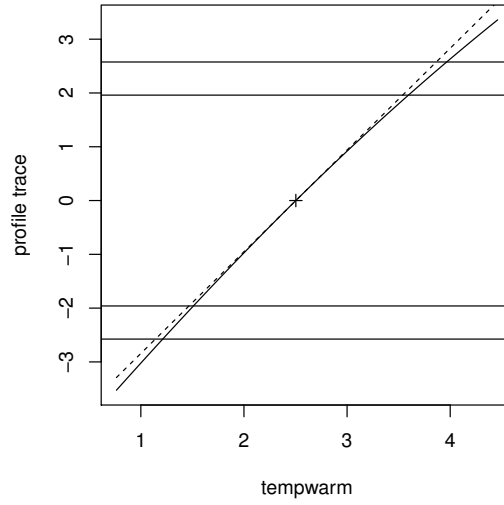


Figure 7: Likelihood root statistic (solid) and Wald statistic (dashed) for the `tempwarm` parameter in the model for the wine data. Horizontal lines indicate 95% and 99% confidence bounds for both statistics.

and provided in Fig. 8. From the relative profile likelihood for `tempwarm` we see that parameter values between 1 and 4 are reasonably well supported by the data, and values outside this range has little likelihood. Values between 2 and 3 are very well supported by the data and all have high likelihood. \square

A An approximate ML estimation method for CLMs

The approach with multiple ordinary logistic regression models considered in example 2 and summarized in Table 2 can be improved on by constructing a single ordinary logistic regression model that estimates the regression parameters only once while also estimating all

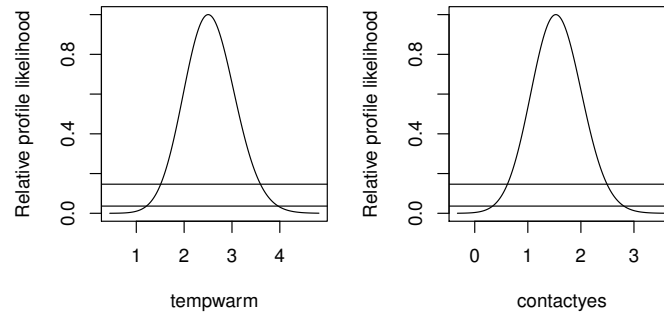


Figure 8: Relative profile likelihoods for the regression parameters in the Wine study. Horizontal lines indicate 95% and 99% confidence bounds.

the threshold parameters. This approach estimates the same parameters as the cumulative logit model, but it does not yield ML estimates of the parameters although generally the estimates are quite close. A larger difference is typically seen in the standard errors which are generally too small. This approach is further described by Winship and Mare (1984).

The basic idea is to form a binary response: $\mathbf{y}^* = [I(\mathbf{y} \leq 1), \dots, I(\mathbf{y} \leq j), \dots, I(\mathbf{y} \leq J - 1)]$ of length $n(J - 1)$, where originally we had n observations falling in J categories. The original design matrix, \mathbf{X} is stacked $J - 1$ times and indicator variables for $j = 1, \dots, J - 1$ are included to give estimates for the thresholds.

Example 20: We now continue example 2 by estimating the parameters with the approach described above. First we form the data set to which we will fit the model:

```
> tab <- with(wine, table(contact, rating))
> dat <- data.frame(freq=c(tab),
                    contact=rep(c("no", "yes"), 5),
                    rating = factor(rep(1:5, each=2), ordered=TRUE))
> dat
```

	freq	contact	rating
1	4	no	1
2	1	yes	1
3	14	no	2
4	8	yes	2
5	13	no	3
6	13	yes	3
7	3	no	4
8	9	yes	4
9	2	no	5
10	5	yes	5

The cumulative link model would be fitted with

```
> fm1 <- clm(rating ~ contact, weights=freq)
```

Then we generate the new response and new data set:

```
> thresholds <- 1:4
> cum.rate <- as.vector(sapply(thresholds, function(x) dat$rating <= x))
> rating.factor <- gl(n=length(thresholds), k=nrow(dat),
                    length=nrow(dat) * length(thresholds))
> thres.X <- model.matrix(~ rating.factor - 1)
> colnames(thres.X) <- paste("t", thresholds, sep="")
> old.X <- -model.matrix(~contact, dat)[, -1, drop=FALSE]
> new.X <- kronecker(matrix(rep(1, length(thresholds)), nc = 1), old.X)
> weights <- kronecker(matrix(rep(1, length(thresholds)), nc = 1), dat$freq)
> new.X <- cbind(thres.X, new.X)
> colnames(new.X)[-seq(length(thresholds))] <- colnames(old.X)
> p.df <- cbind(cum.rate = 1*cum.rate, as.data.frame(new.X), weights)
> p.df
```

	cum.rate	t1	t2	t3	t4	contactyes	weights
1	1	1	0	0	0	0	4
2	1	1	0	0	0	-1	1
3	0	1	0	0	0	0	14
4	0	1	0	0	0	-1	8
5	0	1	0	0	0	0	13
6	0	1	0	0	0	-1	13

7	0	1	0	0	0	0	3
8	0	1	0	0	0	-1	9
9	0	1	0	0	0	0	2
10	0	1	0	0	0	-1	5
11	1	0	1	0	0	0	4
12	1	0	1	0	0	-1	1
13	1	0	1	0	0	0	14
14	1	0	1	0	0	-1	8
15	0	0	1	0	0	0	13
16	0	0	1	0	0	-1	13
17	0	0	1	0	0	0	3
18	0	0	1	0	0	-1	9
19	0	0	1	0	0	0	2
20	0	0	1	0	0	-1	5
21	1	0	0	1	0	0	4
22	1	0	0	1	0	-1	1
23	1	0	0	1	0	0	14
24	1	0	0	1	0	-1	8
25	1	0	0	1	0	0	13
26	1	0	0	1	0	-1	13
27	0	0	0	1	0	0	3
28	0	0	0	1	0	-1	9
29	0	0	0	1	0	0	2
30	0	0	0	1	0	-1	5
31	1	0	0	0	1	0	4
32	1	0	0	0	1	-1	1
33	1	0	0	0	1	0	14
34	1	0	0	0	1	-1	8
35	1	0	0	0	1	0	13
36	1	0	0	0	1	-1	13
37	1	0	0	0	1	0	3
38	1	0	0	0	1	-1	9
39	0	0	0	0	1	0	2
40	0	0	0	0	1	-1	5

where the first column is the new binary response variable, the next four columns are indicator variables for the thresholds, the following column is the indicator variable for **contact** and the last column holds the weights. Observe that while the original data set had 10 rows, the new data set has 40 rows. We fit the ordinary logistic regression model for these data with

```
> glm1 <- glm(cum.rate ~ t1+t2 +t3 +t4 - 1 + contactyes,
               weights=weights, family=binomial, data=p.df)
> summary(glm1)
```

Call:

```
glm(formula = cum.rate ~ t1 + t2 + t3 + t4 - 1 + contactyes,
    family = binomial, data = p.df, weights = weights)
```

Deviance Residuals:

	Min	1Q	Median	3Q	Max
	-4.3864	-1.8412	-0.0202	1.7772	4.7924

Coefficients:

	Estimate	Std. Error	z value	Pr(> z)
t1	-2.14176	0.47616	-4.498	6.86e-06 ***

t2	0.04797	0.29048	0.165	0.86883
t3	1.71907	0.35132	4.893	9.93e-07 ***
t4	2.97786	0.47203	6.309	2.81e-10 ***
contactyes	1.21160	0.33593	3.607	0.00031 ***

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

(Dispersion parameter for binomial family taken to be 1)

Null deviance: 399.25 on 40 degrees of freedom
 Residual deviance: 246.47 on 35 degrees of freedom
 AIC: 256.47

Number of Fisher Scoring iterations: 5

Notice that we suppressed the intercept since the thresholds play the role as intercepts. In comparing these estimates with the estimates from the genuine cumulative logit model presented in the last two columns of Table 2 we see that these approximate ML estimates are remarkably close to the true ML estimates. Observe however that the standard error of the **contact** effect is much smaller; this is due to the fact that the model was fitted to $n(J - 1)$ observations while originally we only had n of those. The weights could possibly be modified to adjust for this, but we will not pursue this any further.

In lack of efficient software that yields ML estimates of the cumulative logit model, this approach could possibly be justified. This might have been the case some 20 years ago. However, in the present situation this approximate approach is only cumbersome for practical applications. \square

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