Count Transformation Models: The cotram Package

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Abstract

The cotram package offers a ready-to-use R implementation of count transformation models, providing a simple but flexible approach for the regression analysis of count responses arising from various, and possibly complex, data-generating processes. In this unified maximum-likelihood framework count models can be formulated, estimated, and evaluated easily. Specific models in the class can be flexibly customised by the choice of the link function and the parameterisation of the transformation function. Interpretation of explanatory variables in the linear predictor is possible at the scales of the discrete odds ratio, hazard ratio, or reverse time hazard ratio, or as conditional mean of transformed counts. The implemented methods for the model class further provide simple tools for model evaluation. The package simplifies the use of transformation models for modelling counts, while ensuring appropriate settings for count data specifically. Extension to the formulated models can be made by the inclusion of response-varying effects, strata-specific transformation functions, or offsets, based on the underlying infrastructure of the tram and mlt R add-on packages, which further ensure the correct handling of the likelihood for censored or truncated observations.

Keywords: conditional distribution function, conditional quantile function, count regression, deer-vehicle collisions, transformation model.

1. Introduction

Count transformation models are a novel model class, offering a flexible and data-driven approach to regressing count data. The diverse set of models in the class, as proposed and discussed in Siegfried and Hothorn (2019), are tailored to analyse count responses from various underlying data-generating processes in a unified maximum-likelihood framework. The R add-on package **cotram** features the implementation of the proposed model class, providing a simple and user-friendly interface to fit and evaluate count transformation models. The package is built using the general infrastructure of the R add-on packages **tram** (Hothorn 2019b) and **mlt** (Hothorn 2018, 2019a) for likelihood-based inference and further extensions to the implemented model specifications.

Count transformation models arise from the direct modelling of the conditional discrete distribution function capturing changes governed by a linear predictor $x^{\top}\beta$. The models in the class can be represented by the general formulation of the conditional distribution function for any y

$$F_{Y|X=x}(y \mid x) = \mathbb{P}(Y \le y \mid x) = F\left(\alpha(\lfloor y \rfloor) - x^{\top}\beta\right), \quad y \in \mathbb{R}^{+}$$
 (1)

with specific models originating from the choice of the different link functions $g = F^{-1}$. The model class includes models with a logit, complementary log-log (cloglog), log-log, and probit link and thus offers interpretability of the linear predictor at various scales. The framework allows evaluating and interpreting the models in a discrete way, while using a computationally attractive, low-dimensional, continuous representation. The models are designed to simultaneously estimate the transformation function α and the regression coefficients β optimising the exact discrete log-likelihood. Simultaneous estimation of the parameters (developed by Hothorn et al. 2018) is performed based on the underlying infrastructure provided by the mlt package (Hothorn 2019a).

All models in the class (1) can be fitted using the general function call

```
R> cotram(<formula>, method = <link>, ...)
```

with formula being any R formula featuring counts as the response and the right hand side as series of terms determining a linear predictor. The specific models in the class can be fitted by choosing one of the link functions for method = link. The set of models specified by the different link functions and the interpretation of the explanatory variables in the linear predictor $x^{\top}\beta$ are outlined in more detail below.

The package further offers predict() and plot() functions to assess and illustrate the estimated linear predictor, conditional distribution and density function, quantiles and the estimated transformation function, both as step-functions and continuously (setting smooth = TRUE). Functionalities for model interpretation and evaluation, such as summary(), coef(), confint(), and logLik() are available in this framework.

2. Discrete Hazards Cox Count Transformation Model

The count transformation model with complementary log-log link function $g = F^{-1}$ (method = "cloglog") offers a discrete version of the Cox proportional hazards model with fully parameterised transformation function α and interpretation of the linear predictor as discrete hazard ratio. The model explains the effects of the exponentiated linear predictor $\exp(-x^{\top}\beta)$ on observed counts as multiplicative changes in discrete hazards $\mathbb{P}(Y = y \mid Y \geq y, x)$, comparing the conditional cumulative hazard function $\log(1 - F_{Y|X=x})$ with the baseline cumulative hazard function $\log(1 - F_Y)$, with $x^{\top}\beta = 0$.

Using the deer-vehicle collisions data from Hothorn *et al.* (2015), we can fit the Cox count transformation model to the roe deer-vehicle collision counts per day, recorded from 2002 to 2011 in Bavaria, Germany, and obtain the estimated multiplicative temporal changes in "risk" as discrete hazards. The tvar variables are sin-cosine transformed times (see Hothorn *et al.* 2015).

To assess how the risk varies across days and seasons, we can now compute the estimated discrete hazards ratio for each day of the year, based on the predictor values of the year 2011. The results, shown in Figure 1, illustrate the changes in the hazard ratios, relative to baseline on January 1st (note that we plot $\exp(\boldsymbol{x}(\text{day})^{\top}\boldsymbol{\beta} - \boldsymbol{x}(2011-01-01)^{\top}\boldsymbol{\beta})$, such that large values correspond to large number of collisions and thus higher risk).

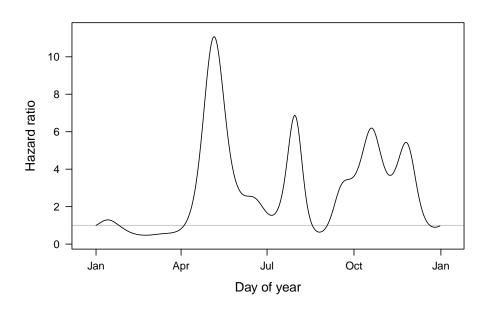


Figure 1: Deer-vehicle collisions. Temporal changes in risk for deer-vehicle collisions across the year as discrete hazard ratios estimated by model mod_cloglog with reference: January 1st. The curve indicates, that the hazard ratio is increased associated with animal activity due to search for new habitats and food resources in April and rut season in July and August. The peak in October does not seem to have a clear explanation in terms of increased roe deer activity.

3. Logistic Count Transformation Model

Odds ratios are often used in practice to compare two different configurations of the set of explanatory variables x. Conveniently, for the class of count transformation models we can obtain the estimated effects on this scale by specifying a logit link. The exponentiated

linear predictor $\exp(-x^{\top}\beta)$ estimated by such a logistic count transformation model can be interpreted as odds ratio

$$\frac{\mathbb{P}(Y \leq y \mid \boldsymbol{x})}{\mathbb{P}(Y > y \mid \boldsymbol{x})} = \frac{\mathbb{P}(Y \leq y)}{\mathbb{P}(Y > y)} \exp(-\boldsymbol{x}^{\top}\boldsymbol{\beta}),$$

comparing the conditional odds of a configuration \boldsymbol{x} with the baseline odds ${}^{F_Y/1-F_Y}$ (with $\boldsymbol{x}^{\top}\boldsymbol{\beta}=0$). The response-varying intercept $\alpha(y)$ cancels out in the odds ratio, resulting in an estimate, which can be interpreted simultaneously across all cut-offs y.

To explain the temporal risk of roe deer-vehicle collisions on the odds ratio scale, the only modification to the model formulation of Section 2 required, is the link specification in the function call as method = "logit".

Comparison of the log-likelihoods of the fitted model and the Cox count transformation model from Section 2 shows almost matching values, with a slight improvement in model fit, when replacing the cloglog with the logit link.

We now could further assess the effect of the factor year on the deer-vehicle collision counts by computing the odds ratios (small values correspond to moving the distribution to the right and thus to larger number of collisions) along with the likelihood-based confidence intervals.

```
R> years <- grep("year", names(coef(mod_logit)), value = TRUE)</pre>
R> coef <- exp(-coef(mod_logit)[years])</pre>
R> ci <- exp(-confint(mod_logit)[years,])</pre>
R> round(cbind(coef, ci), 3)
          coef 2.5 % 97.5 %
year2003 0.595 0.765
                       0.463
year2004 0.337 0.433
                       0.262
year2005 0.305 0.393
                       0.237
year2006 0.406 0.525
                       0.314
year2007 0.156 0.203
                       0.120
year2008 0.096 0.123
                       0.074
year2009 0.104 0.135
                       0.081
year2010 0.090 0.116
                       0.069
year2011 0.097 0.125
                       0.075
```

Plotting the estimated conditional distribution functions of model mod_logit in Figure 2, demonstrates the linear shift in $F_{Y|X=x}$ guided by the different levels of the factor year.

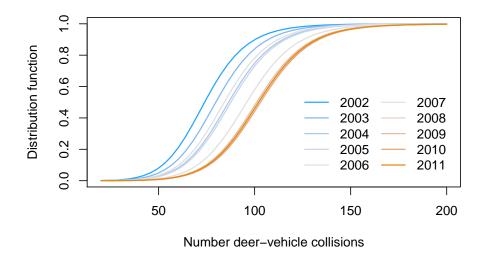


Figure 2: Deer-vehicle collisions. Illustration of the estimated conditional distribution functions of each year between 2002 and 2011.

4. Discrete Reverse Time Hazards Count Transformation Model

Specifying a count transformation model with log-log link $g = F^{-1}$ we get the model formulation

$$F_{Y \mid \boldsymbol{X} = \boldsymbol{x}}(y \mid \boldsymbol{x}) = \mathbb{P}(Y \leq y \mid \boldsymbol{x}) = \exp\left(-\exp\left(\alpha(\lfloor y \rfloor) - \boldsymbol{x}^{\top} \boldsymbol{\beta}\right)\right)$$

with interpretation of the linear predictor $\exp(\boldsymbol{x}^{\top}\boldsymbol{\beta})$ as discrete reverse hazard ratio with multiplicative changes in $\log(F_Y)$. To fit the model, we again only need to adapt the model specification in terms of the link function by setting method = "loglog".

'log Lik.' -16438.23 (df=42)

For further assessment we could evaluate the discrete conditional density of a set of x. Figure 3 illustrates the estimated density function in terms of the predictor values recorded on 2002–01–01 along with the actually observed deer-vehicle collision count.

R> nd <- model.frame(mod_loglog)[1,]</pre>

```
R> plot(mod_loglog, type = "density", newdata = nd, q = 0:150, col = col,
+ xlab = "Number of deer-vehicle collisions", ylab = "Density function")
R> abline(v = nd$DVC)
```

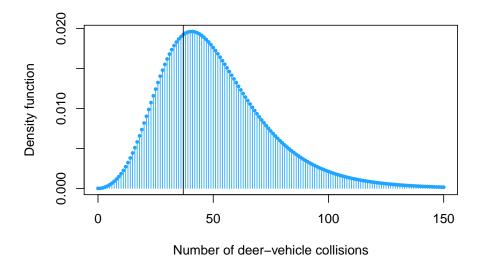


Figure 3: Deer-vehicle collisions. Estimated discrete density function for model mod_loglog with the actual observed count shown as vertical black line.

5. Probit Count Transformation Model

When applying a count transformation model with a probit link (method = "probit") we can interpret the estimated effects as changes in the conditional mean of the transformed counts $\mathbb{E}(\alpha(y) \mid X = x) = x^{\top} \beta$. This interpretation is the same, as obtained from fitting a normal linear regression model on a priori transformed counts, by e.g. a log or square-root transformation. However, for the probit count transformation model, as implemented in the **cotram** package, the transformation of the response y was not heuristically chosen, as in a least-squares approach, but estimated from data by optimising the exact count log-likelihood.

'log Lik.' -16310.32 (df=42)

A simple tool in this framework to check, whether, for example a log transformation, would have been appropriate, is to inspect the estimated transformation function $\alpha(y)$ as illustrated in Figure 4.

```
R> plot(mod_probit, type = "trafo", newdata = df[1,], smooth = TRUE,
+ xlab = "Number of deer-vehicle collisions",
+ ylab = expression(paste("Transformation function ", alpha(y))),
+ col = col[10], lwd = 2)
```

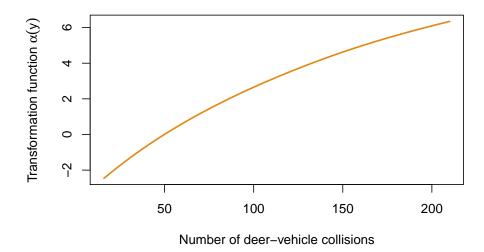


Figure 4: Deer-vehicle collisions. Baseline transformation α estimated by the model mod_probit illustrated as smoothed line.

6. Summary

The implemented models and methods in the **cotram** package offer a unified framework for users to fit and evaluate transformation models for counts, by ensuring the correct handling of the discrete nature of the data. Simplifying the modelling procedure, the models are parameterised under general and empirically tested settings, eliminating the need for overly complicated model specifications.

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Count Transformation Models

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7 Number of words abstract: 349

8 Number of words text: 3738

9 Number of figures: 5

Number of tables: 1

Number of references: 28

Abstract

1. The effect of explanatory environmental variables on a species' distribution is often assessed using a count regression model. Poisson generalised linear models or negative binomial models are common, but the traditional approach of modelling the mean after log or square-root transformation remains popular and in some cases is even advocated.

- 2. We propose a novel class of linear models for count data. Similar to the traditional approach, the new models apply a transformation to count responses; however, this transformation is estimated from the data and not defined a priori. In contrast to simple least-squares fitting and in line with Poisson or negative binomial models, the exact discrete likelihood is optimised for parameter estimation and inference. Interpretation of linear predictors is possible at various scales depending on the model formulation.
- 3. Count transformation models provide a new approach to regressing count data in a distribution-free yet fully parametric fashion, obviating the need to a priori commit to a specific parametric family of distributions or to a specific transformation. The model class is a generalisation of discrete Weibull models for counts and is thus able to handle over- and underdispersion. We demon-

strate empirically that the models are more flexible than Poisson or negative binomial models but still maintain interpretability of multiplicative effects. A re-analysis of deer-vehicle collisions and the results of artificial simulation experiments provide evidence of the practical applicability of the model class.

- 4. In ecology studies, uncertainties regarding whether and how to transform count data can be resolved in the framework of count transformation models, which were designed to simultaneously estimate an appropriate transformation and the linear effects of environmental variables by maximising the exact count log-likelihood. The application of data-driven transformations allows over- and underdispersion to be addressed in a model-based approach. Models in this class can be compared to Poisson or negative binomial models using the in- or out-of-sample log-likelihood. Extensions to non-linear additive or interaction effects, correlated observations, hurdle-type models and other, more complex situations are possible. A free software implementation is available in the cotram add-on package to the R system for statistical computing.
- Keywords conditional distribution function, conditional quantile function,
- count regression, deer-vehicle collisions, transformation model

1 Introduction

Information represented by counts is ubiquitous in ecology. Perhaps the most obvious instance of ecological count data is animal abundances, which 52 are determined either directly, for example by birdwatchers, or indirectly, by 53 the counting of surrogates, for example the number of deer-vehicle collisions as a proxy for roe deer abundance. This information is later converted into models of animal densities or species distributions using statistical models for count data. Distributions of count data are, of course, discrete and rightskewed, such that tailored statistical models are required for data analysis. 58 Here we focus on models explaining the impact of explanatory environmental 59 variables x on the distribution of a count response $Y \in \{0, 1, 2, \dots\}$. In the 60 commonly used Poisson generalised linear model $Y \mid \boldsymbol{x} \sim \text{Po}(\exp(\alpha + \boldsymbol{x}^{\top}\boldsymbol{\beta}))$ with log-link, intercept α and linear predictor $\boldsymbol{x}^{\top}\boldsymbol{\beta}$, both the mean $\mathbb{E}(Y\mid\boldsymbol{x})$ and the variance $\mathbb{V}(Y \mid \boldsymbol{x})$ of the count response are given by $\exp(\alpha + \boldsymbol{x}^{\top}\boldsymbol{\beta})$. 63 Overdispersion, i.e. the situation $\mathbb{E}(Y \mid \boldsymbol{x}) < \mathbb{V}(Y \mid \boldsymbol{x})$, is allowed in the more complex negative binomial model $Y \mid \boldsymbol{x} \sim \text{NB}(\exp(\alpha + \boldsymbol{x}^{\top}\boldsymbol{\beta}), \nu)$ with 65 mean $\mathbb{E}(Y \mid \boldsymbol{x}) = \exp(\alpha + \boldsymbol{x}^{\top}\boldsymbol{\beta})$ and potentially larger variance $\mathbb{V}(Y \mid \boldsymbol{x}) =$ $\mathbb{E}(Y \mid \boldsymbol{x}) + \mathbb{E}(Y \mid \boldsymbol{x})^2 / \nu$. For independent observations, the model parameters 67 are obtained by maximising the discrete log-likelihood function, in which an observation (y, \boldsymbol{x}) contributes the log-density $\log(\mathbb{P}(Y = y \mid \boldsymbol{x}))$ of either the Poisson or the negative binomial distribution.

Before the emergence of these models tailored to the analysis of count data 71 (generalised linear models were introduced by Nelder & Wedderburn 1972), 72 researchers were restricted to analysing transformations of Y by normal linear 73 regression models. Prominent textbooks at the time (Snedecor & Cochran 1967; Sokal & Rohlf 1967) suggested log transformations $\log(y+1)$ or squareroot transformations $\sqrt{y+0.5}$ of observed counts y. The application of leastsquares estimators to the log-transformed counts then leads to the mean $\mathbb{E}(\log(y+1) \mid \boldsymbol{x}) = \alpha + \boldsymbol{x}^{\top}\boldsymbol{\beta}$. Implicitly, it is assumed that the variance after transformation $\mathbb{V}(\log(y+1) \mid \boldsymbol{x}) = \sigma^2$ is constant and that errors 79 are normally distributed. Although it is clear that the normal assumption 80 $\log(Y+1) \mid \boldsymbol{x} \sim N(\alpha + \boldsymbol{x}^{\top}\boldsymbol{\beta}, \sigma^2)$ is incorrect (the count data are still discrete after transformation) and, consequently, that the wrong likelihood is maximised by applying least-squares to $\log(y+1)$ for parameter estimation and 83 inference, this approach is still broadly used both in practice and in theory (e.g. Ives 2015; Dean, Voss & Draguljić 2017; Gotelli & Ellison 2013; De Felipe, Sáez-Gómez & Camacho 2019; Mooney, Phillips, Tillberg, Sandrow, Nelson & Mooney 2016). Moreover, other deficits of this approach have been 87 discussed in numerous papers (e.g. O'Hara & Kotze 2010; Warton, Lyons, Stoklosa & Ives 2016; St-Pierre, Shikon & Schneider 2018; Warton 2018).

As a compromise between the two extremes of using rather strict count dis-

tribution models (such as the Poisson or negative binomial) and the analysis of transformed counts by normal linear regression models, we suggest a novel class of transformation models for count data that combines the strengths of both approaches. Briefly stated, in the newly proposed method appropriate 94 transformations of counts Y are estimated simultaneously with regression coefficients β from the data by maximising the correct discrete form of the likelihood in models that ensure the interpretability of a linear predictor $\boldsymbol{x}^{\top}\boldsymbol{\beta}$ on an appropriate scale. We describe the theoretical foundations of these novel count regression models in Section 2. Practical aspects of the methodology are demonstrated in Section 3 in a re-analysis of roe deer ac-100 tivity patterns based on deer-vehicle collision data, followed by an artificial 101 simulation experiment contrasting the performance of Poisson, negative bi-102 nomial and count transformation models under certain conditions.

$_{\scriptscriptstyle{104}}$ 2 Methods

The core idea of our count transformation model for describing the impact of explanatory environmental variables \boldsymbol{x} on counts $Y \in \{0, 1, 2, ...\}$ is the simultaneous estimation of a fully parameterised smooth transformation $\alpha(Y)$ of the discrete response and the regression coefficients in a linear predictor $\boldsymbol{x}^{\top}\boldsymbol{\beta}$. The aim of the approach is to model the discrete conditional distribu-

tion function $F_{Y|X=x}$ directly.

We develop the novel model starting with a generalised linear model (GLM) for a binary event $Y \leq k$ defined by some cut-off point k. Assuming a Bernoulli distribution $\mathbb{1}(Y \leq k) \sim \mathrm{B}(1, \pi(\boldsymbol{x}))$ with success parameter $\pi(\boldsymbol{x})$, a binary GLM with link function g is given as

$$g(\mathbb{1}(\mathbb{E}(Y \le k \mid \boldsymbol{x}))) = \alpha + \boldsymbol{x}^{\top} \boldsymbol{\beta}.$$

The intercept α defines the probability of a "success" $\mathbb{1}(Y \leq k)$ for a baseline configuration $\boldsymbol{x}^{\top}\boldsymbol{\beta} = 0$ and, in a logistic regression model with g = logit, the regression coefficients $\boldsymbol{\beta}$ have an interpretation as odds ratios $\exp(\boldsymbol{\beta})$.

Now, suppose the maximal possible number of counts Y one can observe is K, so $Y \in \{0, 1, 2, \ldots, K\}$. For this scenario, the binary GLM can be extended to a cumulative model of the form

$$g(\mathbb{1}(\mathbb{E}(Y \le k \mid \boldsymbol{x}))) = \alpha_k + \boldsymbol{x}^{\top} \boldsymbol{\beta}, \quad k = 1, \dots, K - 1$$

as introduced by McCullagh (1980) for ordinal responses. The intercept thresholds α_k are monotonically non-decreasing $\alpha_k \leq \alpha_{k+1}$ and depend on the cut-off point k. With g = logit, the proportional odds logistic regression model is obtained, featuring constant odds ratios $\exp(\boldsymbol{\beta})$ independent of k. For count data, there is usually no such limit K to $\max(Y)$ and thus the number of intercept thresholds α_k may become quite large. The main aspect

of our count transformation models is a smooth and parsimonious parame-129 terisation of the intercept thresholds. To simplify notation, we note that the 130 mean $\mathbb{E}(\mathbbm{1}(Y \leq k \mid \boldsymbol{x})) = \mathbb{P}(Y \leq k \mid \boldsymbol{x})$ has an interpretation as a distribu-131 tion function. Furthermore, each link function $g = F^{-1}$ corresponds to the 132 quantile function of a specific continuous distribution function F (g = logit133 and $F = g^{-1} = \text{expit}$ for logistic regression, $g = \Phi^{-1}$ for probit regression, etc.). Last, using a negative sign for the linear predictor $\boldsymbol{x}^{\top}\boldsymbol{\beta}$ ensures that 135 large values of $\boldsymbol{x}^{\top}\boldsymbol{\beta}$ correspond to large means $\mathbb{E}(Y\mid\boldsymbol{x})$, however, in a non-136 linear way. For arbitrary cut-offs y, we introduce the count transformation 137 model as a model for the conditional distribution function $F_{Y|X=x}(y \mid x)$ of 138 a count response Y given explanatory variables \boldsymbol{x} , as 139

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$$\mathbf{x} = \mathbf{x}(y \mid \mathbf{x}) = \mathbb{P}(Y \le y \mid \mathbf{x}) = F(\alpha(\lfloor y \rfloor) - \mathbf{x}^{\top} \boldsymbol{\beta}), \quad y \in \mathbb{R}^{+}.$$
 (1)

The intercept threshold function $\alpha: \mathbb{R}^+ \to \mathbb{R}$ is now a smooth continuous and monotonically increasing function applied to the greatest integer $\lfloor y \rfloor$ less than or equal to the cut-off point y. Hothorn, Möst & Bühlmann (2018) suggested the parameterisation of α in terms of basis functions $\boldsymbol{a}: \mathbb{R} \to \mathbb{R}^P$ and the corresponding parameters $\boldsymbol{\vartheta}$ as

$$\alpha(y) = \boldsymbol{a}(y)^{\top} \boldsymbol{\vartheta}.$$

The only modification required for count data is to consider this transformation function as a step function with jumps at integers $0, 1, 2, \ldots$ only. This

is achieved in model (1) by the floor function |y|. The very same approach was suggested by Padellini & Rue (2019) but to model quantile functions $F_{Y|X=x}^{-1}$ of count data instead of the distribution functions we consider here. 151 Figure 1 shows a distribution function $F_Y(y) = F(\alpha(\lfloor y \rfloor))$ and the corre-152 sponding transformation function α , both as discrete step-functions (flooring 153 the argument first) and continuously (without doing so). The two versions are identical for integer-valued arguments. Thus, the transformation func-155 tion α , and consequently the transformation model (1), are parameterised 156 continuously but evaluated and interpreted discretely. A computationally attractive, low-dimensional representation of a smooth function in terms of 158 a few basis functions a and corresponding parameters is therefore the core 159 ingredient of our novel model class. In addition to the baseline transforma-160 tion and distribution functions (that is, for a configuration with $\boldsymbol{x}^{\top}\boldsymbol{\beta}=0$ in model (1)), the conditional transformation and distribution function for 162 some configuration $\boldsymbol{x}^{\top}\boldsymbol{\beta}=3$ is also depicted. The impact of $\boldsymbol{x}^{\top}\boldsymbol{\beta}=3$ on the 163 transformation function is given by a vertical shift but is nonlinear on the scale of the distribution function. 165

[Figure 1 about here.]

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On a more technical level, the basis \boldsymbol{a} is specified in terms of $\boldsymbol{a}_{\mathrm{Bs},P-1}$, with P-dimensional basis functions of a Bernstein polynomial (Farouki 2012) of

order P-1. Specifically, the basis a(y) can be chosen as: $a_{Bs,P-1}(y)$ or $m{a}_{\mathrm{Bs},P-1}(y+1),$ or as a Bernstein polynomial on the log-scale: $m{a}_{\mathrm{Bs},P-1}(\log(y))$ or $\mathbf{a}_{Bs,P-1}(\log(y+1))$. The choice of $\mathbf{a}(y) = \mathbf{a}_{Bs,P-1}(\log(y+1))$ is particularly 171 well suited for modelling relatively small counts. For P=1, the defined basis 172 is equivalent to a linear function of either y, $\log(y)$ or $\log(y+1)$. Monotonicity 173 of the transformation function α can be obtained under the constraint $\vartheta_1 \leq$ $\vartheta_2 \leq \cdots \leq \vartheta_P$ of the parameters $\boldsymbol{\vartheta} = (\vartheta_1, \dots, \vartheta_P)^{\top} \in \mathbb{R}^P$ (Hothorn et al. 175 2018). 176 Similar to binary GLMs or cumulative models, specific model types arise from 177 the different a priori choices of the inverse link function $g^{-1} = F : \mathbb{R} \to [0, 1]$. 178 This choice also governs the interpretation of the linear predictor $x^{\top}\beta$. The 179 conditional distribution function $F_{Y|\mathbf{X}=\mathbf{x}}(y \mid \mathbf{x})$ for different choices of the 180 link function $g = F^{-1}$ and any configuration \boldsymbol{x} are given in Table 1, with $F_Y(y) = F(\alpha(\lfloor y \rfloor))$ denoting the distribution of the baseline configuration 182 $\boldsymbol{x}^{\top}\boldsymbol{\beta} = 0$. Note that, with a sufficiently flexible parameterisation of the 183 transformation function $\alpha(y) = \boldsymbol{a}(y)^{\top} \boldsymbol{\vartheta}$, every distribution can be written in this way such that the model is distribution-free (Hothorn et al. 2018). 185 The parameters β describe a deviation from this baseline distribution in 186 terms of the linear predictor $\mathbf{x}^{\top}\boldsymbol{\beta}$. For a probit link, the linear predictor is 187 the conditional mean of the transformed counts $\alpha(Y)$. This interpretation, 188 except for the fact that the intercept is now understood as being part of 189

the transformation function α , is the same as in the traditional approach of 190 first transforming the counts and only then estimating the mean using least-191 squares. However, the transformation α is not heuristically chosen or defined 192 a priori but estimated from data through parameters ϑ , as explained below. 193 For a logit link, $\exp(-\boldsymbol{x}^{\top}\boldsymbol{\beta})$ is the odds ratio comparing the conditional odds 194 $F_{Y|X=x}/1-F_{Y|X=x}$ with the baseline odds $F_{Y}/1-F_{Y}$. The complementary log-log (cloglog) link leads to a discrete version of the Cox proportional hazards 196 model, such that $\exp(-\boldsymbol{x}^{\top}\boldsymbol{\beta})$ is the hazard ratio comparing the conditional 197 cumulative hazard function $\log(1 - F_{Y|X=x})$ with the baseline cumulative hazard function $\log(1 - F_Y)$. The log-log link leads to the reverse time 199 hazard ratio with multiplicative changes in $log(F_Y)$. All models in Table 1 are 200 parameterised to relate positive values of $x^{\top}\beta$ to larger means independent 201 of the specified link $g = F^{-1}$.

[Table 1 about here.]

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In Section 3.1 of our empirical evaluation we consider a linear count transformation model for discrete hazards by specifying the cloglog link. The discrete Cox count transformation model

$$F_{Y|\mathbf{X}=\mathbf{x}}(y \mid \mathbf{x}) = \mathbb{P}(Y \le y \mid \mathbf{x})$$

$$= 1 - \exp\left(-\exp\left(\mathbf{a}_{\mathrm{Bs},P-1}\left(\log(\lfloor y+1 \rfloor)\right)^{\top}\boldsymbol{\vartheta} - \mathbf{x}^{\top}\boldsymbol{\beta}\right)\right)$$
(2)

with P Bernstein basis functions $\boldsymbol{a}_{\mathrm{Bs},P-1}$ relates positive linear predictors

to smaller hazards and thus larger means. The discrete hazard function $\mathbb{P}(Y=y\mid Y\geq y, \boldsymbol{x})$ is the probability that y counts will be observed given that at least y counts were already observed. The model is equivalent to

$$\mathbb{P}(Y = y \mid Y \ge y, \boldsymbol{x}) = \exp(-\boldsymbol{x}^{\top}\boldsymbol{\beta})\mathbb{P}(Y = y \mid Y \ge y)$$

and thus the hazard ratio $\exp(-\boldsymbol{x}^{\top}\boldsymbol{\beta})$ gives the multiplicative change in 214 discrete hazards. 215 The Cox proportional hazards model with a simplified transformation func-216 tion $\alpha(y) = \vartheta_1 + \vartheta_2 \log(y+1)$ specifies a discrete form of a Weibull model 217 (introduced by Nakagawa & Osaki 1975) that Peluso, Vinciotti & Yu (2019) 218 recently discussed as an extension to other count regression models and that 219 serves as a more flexible approach for both over- and underdispersed data. 220 The discrete Weibull model is a special form of our Cox count transformation 221 model (2), as the former features a linear basis function \boldsymbol{a} with P=2 param-222 eters defined by a Bernstein polynomial of order one. Thus, model (2) can be 223 understood as a generalisation moving away from the low-parametric discrete Weibull distribution while maintaining both the interpretability of the effects 225 as log-hazard ratios and the ability to handle over- and underdispersion. 226 Simultaneous likelihood-based inference for ϑ and β for fully parameterised transformation models was developed by Hothorn et al. (2018); here we refer 228 only to the most important aspects. The exact log-likelihood of the model 229

for independent observations $(y_i, \boldsymbol{x}_i), i = 1, \dots, N$ is given by the sum of the N contributions

$$\ell_{i}(\boldsymbol{\vartheta}, \boldsymbol{\beta}) = \log(\mathbb{P}(Y = y_{i} \mid \boldsymbol{x}_{i})) =$$

$$\begin{cases} \log \left[F \left\{ \boldsymbol{a}(0)^{\top} \boldsymbol{\vartheta} - \boldsymbol{x}_{i}^{\top} \boldsymbol{\beta} \right\} \right] & y_{i} = 0 \\ \log \left[F \left\{ \boldsymbol{a}(y_{i})^{\top} \boldsymbol{\vartheta} - \boldsymbol{x}_{i}^{\top} \boldsymbol{\beta} \right\} - F \left\{ \boldsymbol{a}(y_{i} - 1)^{\top} \boldsymbol{\vartheta} - \boldsymbol{x}_{i}^{\top} \boldsymbol{\beta} \right\} \right] & y_{i} > 0. \end{cases}$$

The corresponding log-likelihood is then maximised simultaneously with respect to both ϑ and β under suitable constraints:

$$(\hat{\boldsymbol{\vartheta}}_N, \hat{\boldsymbol{\beta}}_N) = \argmax_{\boldsymbol{\vartheta}, \boldsymbol{\beta}} \sum_{i=1}^N \ell_i(\boldsymbol{\vartheta}, \boldsymbol{\beta}) \quad \text{subject to } \vartheta_p \leq \vartheta_{p+1}, p \in 1, \dots, P-1.$$

Score functions and Hessians are available from Hothorn et al. (2018). The 237 likelihood highlights an important connection to a recently proposed ap-238 proach to multivariate models (Clark, Nemergut, Seyednasrollah, Turner & 239 Zhang 2017), where the main challenge is to make multiple response vari-240 ables measured at different scales comparable. Latent continuous variables are used to model discrete responses by means of appropriate censoring. For the univariate case, considered here, our likelihood is equivalent to censoring 243 a latent continuous variable Y at integers $0, 1, 2, \ldots$ Different choices of 244 the link function g define the latent variable's distribution, e.g. for a probit model with $g = \Phi^{-1}$ a latent normal distribution is assumed.

3 Results

In our empirical evaluation of the proposed count transformation models,
we demonstrate practical aspects of the model class in Section 3.1, by reanalysing data on deer-vehicle collisions, and examine their properties in the
context of conventional count regression models, assuming either a conditional Poisson or a negative binomial distribution. In Section 3.2, we use
simulated count data to evaluate the robustness of count transformation
models under model misspecification.

255 3.1 Analysis of deer-vehicle collision data

In the following, we re-analyse a time series of 341'655 deer-vehicle colli-256 sions involving roe deer (Capreolus capreolus) that were documented between 257 2002-01-01 and 2011-12-31 in Bavaria, Germany. The roe deer-vehicle collisions, recorded in 30-minute time intervals in the whole of Bavaria, were 259 originally analysed by Hothorn, Müller, Held, Möst & Mysterud (2015) with 260 the aim of describing temporal patterns in roe deer activity. The raw data and a detailed description of their analysis are available in the original study. 262 In our re-analysis, we explore the estimates and properties of count regression 263 models explaining how the risk of roe deer-vehicle collisions varies over days (diurnal effects) as well as across weeks, seasons and the whole year. We

applied a Poisson generalised linear model with a log link, a negative binomial model with a log link and a discrete Cox count transformation model (2) with 267 P=7 parameters ϑ of a Bernstein polynomial. The latter two models allow for possible overdispersion. The temporal changes in the risk of roe deer-269 vehicle collisions were modelled as a function of the following explanatory 270 variables: annual, weekly and diurnal effects, an interaction of the weekly and diurnal effects, and seasonal effects, encoded as interactions of diurnal 272 effects with a smooth seasonal component s(d) (based on Held & Paul 2012). 273 The three models were fitted to the data of the first eight years (2002 to 2009) and evaluated based on the data from the remaining two years, 2010 and 2011. 276 For each model we computed the estimated multiplicative seasonal changes 277 in risk depending on the time of day relative to baseline on January 1st, including 95% simultaneous confidence bands. We interpreted "risk" as a 279 multiplicative change to baseline with respect to either the conditional mean 280 ("expectation ratio"; Poisson and negative binomial models) or the conditional discrete hazard function ("hazard ratio") for the Cox count transfor-282 mation model (2).

[Figure 2 about here.]

The results in Figure 2 show a rather strong agreement between the three

283

284

models with respect to the estimated risk (expectation ratio or hazard ratio). However, the uncertainty, assessed by the 95% confidence bands, was under-287 estimated in the Poisson model. The negative binomial and the Cox count transformation model (2) agree on the effects and the associated variability, 289 with the possible exception of the risk at daylight (Day, am). 290 To assess the performance of the three count regression models, we computed the out-of-sample log-likelihoods of each model based on the data of the 292 validation sample (year 2010 and 2011). The out-of-sample log-likelihood of 293 the Cox count transformation model (2) with a value of -58'164.47 was the largest across the three count regression models. The Poisson model, with an out-of-sample log-likelihood of -67'192.75, was the most inconsistent with 296 the data. Allowing for possible overdispersion by the negative binomial model 297 increased the out-of-sample log-likelihood to -58'234.72, which was closer to but did not match the out-of-sample log-likelihood of model (2). Practically, 299 the count transformation model performed as good as the negative binomial 300 model, however, the necessity to choose a specific parametric distribution was present in the latter model only owing to the distribution-free nature of 302 the former. 303 We further compared the three different models in terms of their conditional distribution functions for four selected time intervals of the year 2009. The

discrete conditional distribution functions of the models, evaluated for all

integers between 0 and 38, are given in Figure 3. The conditional medians
obtained from all three models are rather close, but the variability assessed
by the Poisson model is much smaller than that associated with the negative
binomial and count transformation models, thus indicating overdispersion.

[Figure 3 about here.]

3.2 Artificial count-data-generating processes

311

We investigated the performance of the different regression models in a simulation experiment based on count data from various underlying data-314 generating processes (DGPs). Count responses Y were generated condition-315 ally on a numeric predictor variable $x \in [0,1]$ following a Poisson or negative binomial distribution or one of the discrete distributions underlying the four 317 count transformation models corresponding to the four link functions from 318 Table 1. For the Poisson model, the mean and variance were assumed to be $\mathbb{E}(Y\mid x) = \mathbb{V}(Y\mid x) = \exp(1.2 + 0.8x)$. The negative binomial data were chosen to be moderately overdispersed, with $\mathbb{E}(Y \mid x) = \exp(1.2 + 0.8x)$ and 321 $\mathbb{V}(Y\mid x) = \mathbb{E}(Y\mid x) + \mathbb{E}(Y\mid x)^2/3$. The four data-generating processes 322 arising from the count transformation models were specified by the different link functions in Table 1, a Bernstein polynomial $a_{Bs,6}(\log(y+1))$ and a 324 regression coefficient $\beta_1 = 0.8$.

We repeated the simulation experiment for each count-data-generating process 100 times, with learning and validation sample sizes of N=250 and $\tilde{N}=750$ respectively. The centred out-of-sample log-likelihoods, contrasting the model fit, were computed by the differences between the out-of-sample log-likelihoods of the models and the out-of-sample log-likelihoods of the true generating processes.

[Figure 4 about here.]

The results as given in Figure 4 follow a clear pattern. When misspecified, 333 the model fit of the Poisson model is inferior to that of all other models. As 334 expected, the negative binomial model well fits both the data arising from 335 the Poisson distribution (limiting case of the negative binomial distribution 336 with $\nu \to \infty$) and the moderately overdispersed data. However, it lacks ro-337 bustness for more complex data-generating processes, such as the underlying mechanisms specified by a count transformation model. The fit of the count 339 transformation models is satisfactory across all DGPs, albeit with some dif-340 ferences within the model class. 341

4 Discussion

332

Motivated by the challenges posed by the statistical analysis of ecological count data, we present a novel class of count transformation models that

provide a unified approach tailored to the analysis of count responses. The 345 model class, as outlined in Section 2, offers a diverse set of count models and can be specified, estimated and evaluated in a simple but flexible maximum 347 likelihood framework. The direct modelling of the conditional discrete distri-348 bution, while preserving the interpretability of the linear predictor $x^{\top}\beta$, is 349 a key feature of our count transformation model. Furthermore, it eliminates the need to impose restrictive distributional assumptions, to choose transfor-351 mations in a data-free manner or to rely on rough approximations of the exact 352 likelihood. The models are flexible enough to handle different dispersion lev-353 els adaptively, without being restricted to either over- or underdispersion. 354 Our results from the re-analysis of deer-vehicle collision data, presented in 355 Section 3.1, demonstrate the favourable properties of count transformations 356 in practice. They are especially compelling for the analysis of count responses arising from more complex data-generating processes, for which the Poisson 358 and even the more flexible negative binomial distribution are of limited use 359 (as illustrated in Section 3.2). Moreover, conditional quantiles can be easily extracted from the fitted model by numerical inversion of the smooth con-361 ditional distribution function $F(\alpha(y) - \boldsymbol{x}^{\top}\boldsymbol{\beta})$. An additional advantage of 362 count transformation models is that the model class allows researchers to flexibly choose the scale of the interpretation of the linear predictor $x^{\top}\beta$ by specifying a link function $g = F^{-1}$ from Table 1.

The model class can be easily tailored to the experimental design using strata-366 specific transformation functions $\alpha(|y|| \text{ strata})$ or response-varying effects $\beta(|y|)$. Correlated observations arising from clustered data require the inclusion of random effects with subsequent application of a Laplace approxi-369 mation to the likelihood. Accounting for varying observation times or batch 370 sizes is straightforward by the inclusion of an offset in the model specification. Random censoring is easy to incorporate in the likelihood (Hothorn 372 et al. 2018), which can then appropriately handle uncertain recordings (for 373 example, the observation "more than three roe-deer vehicle collisions in half an hour" corresponds to right-censoring at three). The same applies to trun-375 cation. By contrast, hurdle-like transformation models require modifications 376 of the basis functions as well as interactions between the response and ex-377 planatory variables (see Section 4.5 in Hothorn et al. 2018). Extensions to the proposed simple shift count transformation model can be 379 made by boosting algorithms (Hothorn 2019b) that allow the estimation of 380 conditional transformation models (Hothorn, Kneib & Bühlmann 2014) featuring complex, non-linear, additive or completely unstructured tree-based 382 conditional parameter functions $\vartheta(x)$. Similarly, count transformation mod-383 els can be partitioned by transformation trees (Hothorn & Zeileis 2017), 384 which in turn lead to transformation forests, as a statistical learning approach for computing predictive distributions. The transformation approach 386

seems also promising for the development for multivariate species distribution 387 models, because different marginal transformation models can be combined 388 into a multivariate model on the same scale (the idea was developed for continuous responses by Klein, Hothorn & Kneib 2019, and recent research 390 focuses on discrete or count variables). 391 The greatest challenge in applying count transformation models is their interpretability. The effects of the explanatory environmental variables are not 393 directly interpretable as multiplicative changes in the conditional mean of the 394 count response, as is the case in Poisson or negative binomial models with a log link. For the logit, cloglog and log-log link functions, the effects are still 396 multiplicative, but at the scales of the discrete odds ratio, hazard ratio or 397 reverse time hazard ratio, which might be difficult to communicate to prac-398 titioners. If the probit link is used, the effects are interpretable as changes in the conditional mean of the transformed counts. This interpretation is the 400 same as that obtained from running a normal linear regression model on, for 401 example, log-transformed counts, with the important difference that (i) the transformation was estimated from data by optimising (ii) the exact discrete 403 likelihood. Nonetheless, it is possible to plot the estimated transformation 404 function $\mathbf{a}(y)^{\top}\hat{\boldsymbol{\vartheta}}$ against $\log(y+1)$ ex post to assess the appropriateness of 405 applying a log-transformation.

of Computational details

418

All computations were performed using R version 3.6.1 (R Core Team 2019). 408 A reference implementation of transformation models is available in the **mlt** 409 R add-on package (Hothorn 2019a; 2018). A simple user interface to lin-410 ear count transformation models is available in the cotram add-on package 411 (Siegfried & Hothorn 2019). The package includes a introductory vignette 412 and reproducibility material for the empirical results presented in Section 3. The following example demonstrates the functionality of the **cotram** pack-414 age in terms of a count transformation model with a cloglog link explaining 415 how the number of tree pipits (Anthus trivialis) varies across different percentages of canopy overstorey cover (coverstorey). 417

```
### package cotram available from CRAN.R-project.org
### install.packages(c("cotram", "coin"))
library("cotram")
### tree pipit data; doi: 10.1007/s10342-004-0035-5
data("treepipit", package = "coin")
### fit discrete Cox model to tree pipit counts
m <- cotram(counts ~ coverstorey, ### log-hazard ratio of
                                  ### coverstorey
            data = treepipit,
                                  ### data frame
            method = "cloglog",
                                 ### link = cloglog
            order = 5,
                                  ### order of Bernstein poly.
            prob = 1)
                                  ### support is 0...5
                                   ### log-likelihood
logLik(m)
## 'log Lik.' -38.27244 (df=7)
exp(coef(m))
                                   ### hazard ratio
## coverstorey
     0.9805453
exp(confint(m))
                                   ### 95% confidence interval
                   2.5 %
                          97.5 %
##
## coverstorey 0.9697581 0.9914526
### more illustrations
# vignette("cotram", package = "cotram")
```

- The data are shown in Figure 5 overlayed with the smoothed version of the
- estimated conditional distribution functions for varying values of coverstorey.

[Figure 5 about here.]

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Link F^{-1}	Interpretation of $\boldsymbol{x}^{\top}\boldsymbol{\beta}$
probit	$\mathbb{E}(lpha_Y(Y) \mid \boldsymbol{x}) = \boldsymbol{x}^{ op} \boldsymbol{\beta}$
logit	$rac{F_{Y oldsymbol{X}=oldsymbol{x}}(y oldsymbol{x})}{1-F_{Y oldsymbol{X}=oldsymbol{x}}(y oldsymbol{x})} = \exp(-oldsymbol{x}^{ op}oldsymbol{eta}) rac{F_{Y}(y)}{1-F_{Y}(y)}$
cloglog	$1 - F_{Y \boldsymbol{X} = \boldsymbol{x}}(y \mid \boldsymbol{x}) = (1 - F_Y(y))^{\exp(-\boldsymbol{x}^\top \boldsymbol{\beta})}$
loglog	$F_{Y \boldsymbol{X}=\boldsymbol{x}}(y\mid \boldsymbol{x}) = F_Y(y)^{\exp(\boldsymbol{x}^\top\boldsymbol{\beta})}$

Table 1: Transformation Model. Interpretation of linear predictors $\boldsymbol{x}^{\top}\boldsymbol{\beta}$ under different link functions $g=F^{-1}$.

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546		than 0.65, the probability of observing at most one tree pipit	
547		is somewhat larger than 0.70. For a coverstorey of 60%, the	
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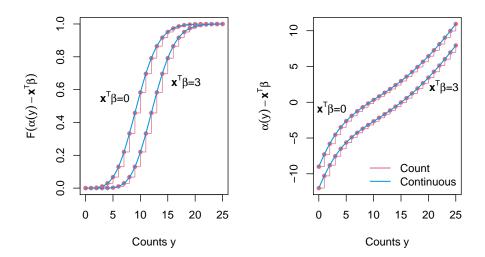


Figure 1: Transformation model. Illustration of a cumulative distribution function (F, left panel) and of a transformation function $(\alpha, \text{ right panel})$ of a count response $(\lfloor y \rfloor, \text{ red})$ and a corresponding continuous variable (y, blue), both functions coinciding for counts $0, 1, 2, \ldots$. The curves are shown both for the baseline configuration $\boldsymbol{x}^{\top}\boldsymbol{\beta} = 0$ and a configuration $\boldsymbol{x}^{\top}\boldsymbol{\beta} = 3$ governing a vertical shift on the scale of the transformation function α (right panel) and corresponding change on the scale of the distribution function (left panel).

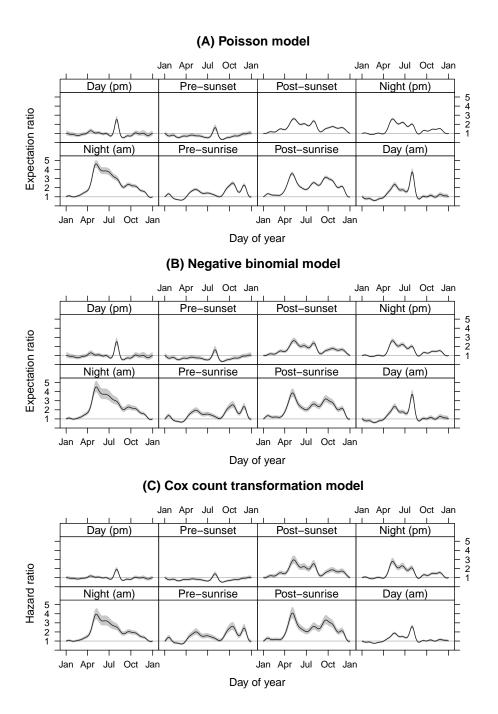


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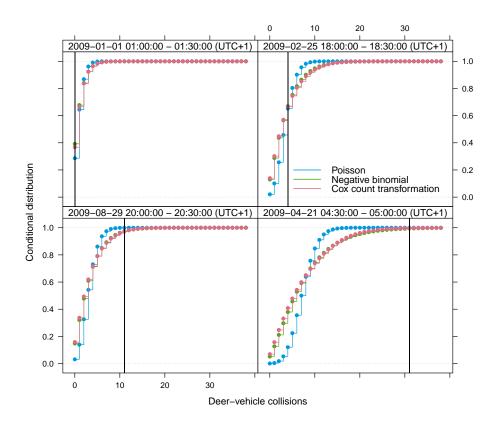


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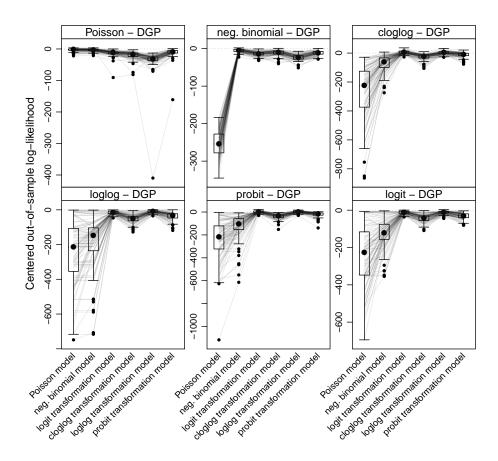


Figure 4: Artificial count-data-generating processes (DGPs). The performance of the count regression models (Poisson, negative binomial and count transformation models outlined in Table 1) assessed by the centered out-of-sample log-likelihood of the corresponding model. Larger values of the out-of-sample log-likelihood indicate a better performance of the corresponding count regression model.

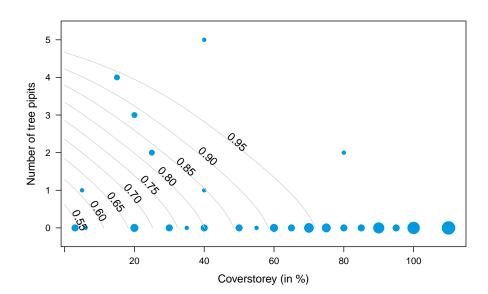


Figure 5: Tree pipit illustration. Number of tree pipits counted at 86 different plots with varying coverstorey. The sizes of the circles are proportional to the square-root of the sample size. Observations are overlayed with the smoothed conditional distribution functions. For a coverstorey of 20%, for example, the probability of not observing any tree pipit is slightly larger than 0.65, the probability of observing at most one tree pipit is somewhat larger than 0.70. For a coverstorey of 60%, the probability of observing at least one tree pipit is less than 0.1.

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