

# Two-stage approaches to the analysis of occupancy data II. The heterogeneous model and conditional likelihood

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## Abstract

Occupancy models involve both the probability a site is occupied and the probability occupancy is detected. The homogeneous occupancy model, where the occupancy and detection probabilities are the same at each site, admits an orthogonal parameter transformation that yields a two-stage process to calculate the maximum likelihood estimates so that it is not necessary to simultaneously estimate the occupancy and detection probabilities. The two-stage approach is examined here for the heterogeneous occupancy model where the occupancy and detection probabilities now depend on covariates that may vary between sites and over time. There is no longer an orthogonal transformation but this approach effectively reduces the parameter space and allows fuller use of the R functionality. This permits use of existing vector generalised linear models methods to fit models for detection and allows the development of an iterative weighted least squares approach to fit models for occupancy. Efficiency is examined in a simulation study and the full

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maximum likelihood and two-stage approaches are compared on several data sets.<sup>1</sup>

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## 1. Introduction

Occupancy models were introduced in MacKenzie et al. (2002). They model the probability a site is occupied and the probability that occupancy is detected. We assume here that occupancy of a site is permanent over the observation period. Data are collected over repeated visits to a number of sites and consist of observations on whether occupancy is detected. It is common that both the occupancy and detection probabilities are modelled in terms of covariates, which can be time varying. Occupancy is related to time independent site covariates and detection can be related to both these site covariates and the time varying covariates. Thus modelling detection can be more complex than modelling occupancy.

Occupancy models are currently fitted to data using the full likelihood where the parameters associated with occupancy and detection are simultaneously estimated. The likelihood may be maximised numerically using the R Development Core Team (2018) package `unmarked` (Fiske and Chandler, 2015) for example. We have observed that the full likelihood can be numerically unstable. This is distinct from boundary solutions that occur in occupancy models, as noted in Wintle et al. (2004); Guillera-Aroita et al. (2010); Karavarsamis et al. (2013); Hutchinson et al. (2015b). Without con-

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<sup>1</sup>Software appears as annexes in the electronic version of this manuscript.

straints, the full likelihood may not converge, may give local maxima, or give estimates beyond the boundaries of the parameter space. Using the common logit transformation can still give estimated probabilities that are effectively zero or one. We examine this in simulations in Section 4 where it is seen that maximum likelihood can give extreme estimates of occupancy parameters when the two-stage approach does not.

Bayesian methods have been developed to estimate occupancy and detectability, for example Milne et al. (1989); Lunn et al. (2000); Wintle et al. (2003); MacKenzie et al. (2006); Gimenez et al. (2007); Royle and Dorazio (2008); Gimenez et al. (2009); MacKenzie et al. (2009); Fiske and Chandler (2011); Martin et al. (2011); Aing et al. (2011); Hui et al. (2011). An empirical Bayes method is known but this can underestimate the variance of the posterior distribution (Royle and Dorazio, 2008; Fiske and Chandler, 2011). Penalized likelihood methods for occupancy have also been developed to help overcome the numerical instability of the maximum likelihood estimators (Moreno and Lele, 2010; Hutchinson et al., 2015b). These may be fitted using the `occuPEN` and `occuPEN_CV` functions in `unmarked` package. In our two-stage approach we address potential instability by considering detection and occupancy separately. This allows us to compute the estimates over two lower dimension parameter spaces. Moreover, the more complex modelling of the effect of time dependent covariates on the detection probabilities is relatively straightforward in the two-stage approach.

To help stabilise the numerical optimization algorithm the package `unmarked`

(see p. 2 of the R vignette Fiske and Chandler (2015)<sup>2</sup>) recommends that covariates be standardized. However, as observed in the documentation for the `unmarked` package, standardizing may cause problems with standard R functions, such as `predict`. The `smartpred` package may solve some issues but not in all instances of data dependent parameters. Moreover, there is no guarantee that users will standardise their data. In addition, the choice of algorithm for the numerical maximisation may be changed in `optim`, however this may be sensitive to the algorithm used.

Recently Karavaarsamis and Huggins (2017) showed that for the homogeneous occupancy model a simple transformation yielded orthogonal parameters resulting in a two-stage estimation procedure that simplified the computation of the estimates. We see in Section 3 that this no longer holds for heterogeneous models. Following the homogeneous case, a conditional likelihood is used to estimate detection probabilities which is the first stage of the analysis. This may be implemented using the `vglm` function in the `VGAM` package in R (Yee, 2010, 2015; Yee et al., 2015). In the second stage, the remaining partial likelihood, evaluated at the estimated detection probabilities from the first stage, is used to estimate the occupancy probabilities. This effectively reduces the parameter space and allows the use of vector generalized linear model methods to fit models for detection. The partial likelihood for occupancy may be maximised using several numerical methods, here we implement this using an iterative weighted least squares (IWLS) approach.

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<sup>2</sup>[cran.at.r-project.org/web/packages/unmarked/vignettes/unmarked.pdf](http://cran.at.r-project.org/web/packages/unmarked/vignettes/unmarked.pdf)

Our notation is given and the full likelihood is examined in Section 2. In Section 3 we describe the two-stage approach. In the first stage in Section 3.1 we use conditional likelihood to estimate the detection probabilities, with time independent detection probabilities discussed in Section 3.1.1 and time dependent detection probabilities considered in Section 3.1.2. In the second stage in Section 3.2 we introduce a partial likelihood approach to estimate the occupancy probabilities using the detection probabilities estimated in the first stage. In Section 3.2.1 we give an IWLS algorithm to compute the occupancy estimates. A simulation study is conducted in Section 4 and the methods are applied to several data sets in Section 5. Some discussion is given in Section 6. Some technical derivations and the implementation of `vglm` in this setting are given in the appendices.

## 2. Notation and Full Likelihood

Consider  $S$  sites labelled  $s = 1, \dots, S$  and  $\tau$  occasions at each site where the presence of a species may be observed. We suppose that occupancy is constant over the observation period. Let  $\psi_s$  be the probability that site  $s$  is occupied and  $p_{sj}$  be the probability the species is observed at site  $s$  on visit  $j$  given it is present at site  $s$ . Then  $\theta_s = 1 - \prod_{j=1}^{\tau} (1 - p_{sj})$  is the probability of at least one detection at site  $s$  given the site is occupied. If there is no dependence on the visit then  $p_{sj} = p_s$  and  $\theta_s = 1 - (1 - p_s)^\tau$ . Let  $Y_{sj}$  take the value 1 if an individual was detected at site  $s$  on occasion  $j$  and zero otherwise. Let  $Y_s = \sum_{j=1}^{\tau} y_{sj}$  denote the number of occasions upon which the species was detected at site  $s$ . We let  $Z_s = I(y_s = 0)$  be the indicator of no detections at site  $s$ . Reorder the  $S$  sites  $s = 1, \dots, O, O + 1, \dots, S$ ,

where  $1, \dots, O$  denote the sites at which at least one detection occurred and  $O + 1, \dots, S$  the remainder sites at which no sightings occurred.

It is common for covariates that may be related to detection or occupancy to be associated with each site. Suppose that  $\psi_s = h(x_s^T \boldsymbol{\alpha})$  where  $x_s$  is a vector of covariates associated with site  $s$  and  $\boldsymbol{\alpha} \in \mathbb{R}^p$  is a vector of coefficients. Let  $p_{sj}$  be the probability of detection at site  $s$  on occasion  $j$  if site  $s$  is occupied. We take  $p_{sj} = h(u_{sj}^T \boldsymbol{\beta})$  where  $u_{sj}$  is a vector of covariates associated with site  $s$  on occasion  $j$ , and let  $\theta_s = 1 - \prod_{j=1}^{\tau} (1 - p_{sj})$ , for site and time dependent detection. For time independent detection probabilities, we write  $p_{sj} = p_s = p(u_s, \boldsymbol{\beta}) = h(u_s^T \boldsymbol{\beta})$ ,  $j = 1, \dots, \tau$ , for a possibly different vector of covariates  $u_s$  to that above and with corresponding coefficient vector  $\boldsymbol{\beta} \in \mathbb{R}^q$ . In most applications  $h$  will be the logistic function  $h(x) = (1 + \exp(-x))^{-1}$ . Let  $\mathbf{p}_s = (p_{s1}, \dots, p_{s\tau})^T$  in the time dependent case and  $\mathbf{p}_s = p_s$  otherwise.

The contribution to the full likelihood of site  $s$ , can be written as

$$L_s(\psi_s, \mathbf{p}_s) = (1 - \psi_s \theta_s)^{z_s} \left\{ \psi_s \prod_{j=1}^{\tau} p_{sj}^{y_{sj}} (1 - p_{sj})^{1 - y_{sj}} \right\}^{1 - z_s}. \quad (1)$$

The full likelihood is based on maximising the product of (1) over all the sites. Let

$$\begin{aligned} \ell(\psi_s, \mathbf{p}_s) &= z_s \log(1 - \psi_s \theta_s) + (1 - z_s) \log(\psi_s) \\ &\quad + (1 - z_s) \sum_{j=1}^{\tau} y_{sj} \log(p_{sj}) + (1 - z_s) \sum_{j=1}^{\tau} (1 - y_{sj}) \log(1 - p_{sj}) \end{aligned}$$

be the contribution of site  $s$  to the log-likelihood. Then, assuming sites are independent, the full log-likelihood is  $\ell(\boldsymbol{\alpha}, \boldsymbol{\beta}) = \sum_{s=1}^S \ell(\psi_s, \mathbf{p}_s)$ .

### 3. The Two-Stage Approach

Following the homogeneous case of Karavarsamis and Huggins (2017) an alternate approach is to let  $\eta_s (= \psi_s \theta_s)$  be the unconditional probability the species is detected at site  $s$ . Then we may write the contribution of site  $s$  to the full likelihood, (1), as

$$\begin{aligned} L(\eta_s, \mathbf{p}_s) &= (1 - \eta_s)^{z_s} \eta_s^{1-z_s} \times \left\{ \frac{\prod_{j=1}^{\tau} p_{sj}^{y_{sj}} (1 - p_{sj})^{1-y_{sj}}}{\theta_s} \right\}^{1-z_s} \\ &= L_1(\eta_s) L_2(\mathbf{p}_s). \end{aligned} \quad (2)$$

The partial likelihood component  $L_1(\eta_s)$  is a Bernoulli likelihood corresponding to the detection of the species at site  $s$  and the partial component  $L_2(\mathbf{p}_s)$  is the conditional likelihood of  $\mathbf{p}_s$  given at least one detection at the site. The contribution of site  $s$  to the log-likelihood is then

$$\begin{aligned} \ell(\eta_s, \mathbf{p}_s) &= z_s \log(1 - \eta_s) + (1 - z_s) \log(\eta_s) \\ &+ (1 - z_s) \left\{ \sum_{j=1}^{\tau} y_{sj} \log(p_{sj}) + \sum_{j=1}^{\tau} (1 - y_{sj}) \log(1 - p_{sj}) - \log(\theta_s) \right\}. \end{aligned} \quad (3)$$

Our interest is in exploiting the decomposition (2) to simplify the calculations for complex models. To achieve this, we use (4) to estimate  $\boldsymbol{\beta}$  in the first stage of the estimation process. Let  $\widehat{\boldsymbol{\beta}}$  be the resulting conditional likelihood estimator of  $\boldsymbol{\beta}$ , and denote its large sample variance by  $V_{\boldsymbol{\beta}}$ . In the second stage, let  $\widehat{\mathbf{p}}_s$  be the fitted value of  $\mathbf{p}_s$  and  $\widehat{\theta}_s$  the fitted value of  $\theta_s$ . We then replace  $\eta_s$  by  $\widetilde{\eta}_s = \psi_s \widehat{\theta}_s$  in the log-partial likelihood (3) and maximise this to estimate  $\boldsymbol{\alpha}$ .

From (4) the conditional likelihood estimator of  $\boldsymbol{\beta}$  arises from solving

$$0 = S_1(\boldsymbol{\beta}) = \sum_{s=1}^S \frac{\partial \ell(\eta_s, \mathbf{p}_s)}{\partial \mathbf{p}_s^T} \frac{\partial \mathbf{p}_s^T}{\partial \boldsymbol{\beta}}. \quad (5)$$

Rather than solving (5) the maximum likelihood estimators of  $\boldsymbol{\beta}$  arise from solving

$$\begin{aligned} 0 &= \sum_{s=1}^S \frac{\partial \ell(\eta_s, \mathbf{p}_s)}{\partial \boldsymbol{\beta}} \\ &= \sum_{s=1}^S \left\{ \frac{\partial \ell(\eta_s, p_s)}{\partial \eta_s} \frac{\partial \eta_s}{\partial \mathbf{p}_s^T} + \frac{\partial \ell(\eta_s, p_s)}{\partial \mathbf{p}_s^T} \right\} \frac{\partial \mathbf{p}_s^T}{\partial \boldsymbol{\beta}} \\ &= \sum_{s=1}^S \frac{\partial \ell(\eta_s, p_s)}{\partial \eta_s} \frac{\partial \eta_s}{\partial \mathbf{p}_s^T} + S_1(\boldsymbol{\beta}). \end{aligned}$$

Thus unlike the simple homogeneous model considered in Karavarsamis and Huggins (2017) the conditional likelihood estimators will not be the mle's.

### 3.1. Stage 1: Estimating the Detection Probabilities

For the homogeneous model Karavarsamis and Huggins (2017) included in their supplementary materials a plot of the estimated occupancy probability against values of the detection probability. This plot suggests that the occupancy probability is relatively insensitive to small changes in the detection probability. Thus modelling the detection probability may not be crucial. However, particularly if there are big changes in the detection probabilities between visits, correct modelling will be expected to improve the estimates and may be of interest independent to  $\psi$ .

### 3.1.1. Time Independent Detection Probabilities

This is the simplest case, apart from constant detection probability. In this case  $\mathbf{p}_s = p_s$  and the conditional likelihood reduces to

$$L_2(\boldsymbol{\beta}) = \prod_{s=1}^O \frac{p_s^{y_s} (1 - p_s)^{\tau - y_s}}{\theta_s},$$

which is a function of the number of detections at each site where there was at least one detection, i.e.  $y_s, s = 1, \dots, O$ . This is the conditional likelihood of Huggins (1989) which may be easily maximised using the **VGAM** package, with nomenclature similar to that used in generalised linear models (§17.2 Yee, 2015; Yee et al., 2015). See Appendix A, Appendix A.1 and Section 5 for details and examples.

### 3.1.2. Time Dependent Detection Probabilities

Recall that in this case we have distinct probabilities  $p_{sj}, j = 1, \dots, \tau$  for different visits to site  $s$ . A simple extension of the time independent model allows an effect of the  $j$ th visit in the model for  $p_{sj}$ . That is, the covariate vector  $u_{sj}$  contains an indicator of the visit time. This is modelled by allowing the intercept to vary with the visit, and this is easily implemented in the **VGAM** package. See Appendix A.2 and Section 5. More generally environmental variables such as temperature or the time of day the visit was conducted may vary between visits. When we allow the detection probabilities to depend on time dependent covariates, the conditional likelihood corresponding to a site  $s$  where occupancy was detected is now

$$L_2(\mathbf{p}_s) = \frac{\prod_{j=1}^{\tau} p_{sj}^{y_{sj}} (1 - p_{sj})^{1 - y_{sj}}}{\theta_s}.$$

That is, the detections form a sequence of independent Bernoulli trials but we only observe the outcome if there is at least one detection. Again this model can be fitted using the VGAM package. See Appendix A.2 for details.

### 3.2. Stage 2: Estimating Occupancy Probabilities

To estimate  $\boldsymbol{\alpha}$  we maximise the partial likelihood  $\prod_{s=1}^S L_{1s}(\tilde{\eta}_s)$  where, as noted above,  $\mathbf{p}_s$  and hence  $\theta_s$  has been replaced by its estimator from the first stage  $\hat{p}_s = \mathbf{p}_s(\hat{\boldsymbol{\beta}})$ . The partial likelihood is  $L_1(\boldsymbol{\alpha}) = \prod_{s=1}^S L_{1s}(\tilde{\eta}_s) \propto \prod_{s=1}^S (1 - \psi_s \hat{\theta}_s)^{z_s} \psi_s^{1-z_s}$ . Let  $w_s = 1 - z_s$ , then the log-partial likelihood is

$$\ell(\boldsymbol{\alpha}) = \sum_{s=1}^S \left\{ (1 - w_s) \log(1 - \psi_s \hat{\theta}_s) + w_s \log(\psi_s) \right\}. \quad (6)$$

This may be maximised numerically using the `optim` function in R (referred to as ‘‘Partial’’ in tables). However, there are two other possible approaches.

#### 3.2.1. Iterative Weighted Least Squares

An alternative to this method that is commonly used to compute estimates from generalised linear models is the well known iterative weighted least squares (IWLS) approach. To define this estimator for a logistic model, let the matrix  $X$  have  $s$ th column  $x_s$ . Let  $\mathbf{w} = (w_1, \dots, w_S)^T$ ,  $\eta_s = \theta_s \psi_s$ ,  $\boldsymbol{\eta} = (\eta_1, \dots, \eta_S)^T$ . Let  $\boldsymbol{\eta}(\boldsymbol{\alpha})$  be  $\boldsymbol{\eta}$  evaluated at  $\boldsymbol{\alpha}$ . Set  $V = \text{diag}\{(1 - \boldsymbol{\eta})\boldsymbol{\eta}\}$  and  $U = \text{diag}\{\theta_s \psi_s (1 - \psi_s)\}$ . Let  $\boldsymbol{\alpha}^{(k)}$  be the estimate at the  $k$ th step and let  $\mathbf{Z} = UX\boldsymbol{\alpha}^{(k)} + \mathbf{w} - \boldsymbol{\eta}(\boldsymbol{\alpha}^{(k)})$ . Then the estimate at the  $(k + 1)$ th is  $\boldsymbol{\alpha}^{(k+1)} = (XUV^{-1}UX^T)^{-1}XUV^{-1}U\mathbf{Z}$ . The IWLS estimate is obtained by repeating this step until convergence. Details are given in Appendix B. An estimate of the expected Fisher information corresponding to the partial likelihood,  $E\{I(\boldsymbol{\alpha}, \boldsymbol{\beta})\}$ , is given by  $\tilde{I}(\boldsymbol{\alpha}, \boldsymbol{\beta}) = XUV^{-1}UX^T$ .

### 3.2.2. Iterative Offset

As  $\theta_s$  does not depend on  $\boldsymbol{\alpha}$ , maximising (6) is equivalent to maximising

$$\ell(\boldsymbol{\alpha}) = \sum_{s=1}^S \{(1 - w_s) \log(1 - \hat{\eta}_s) + w_s \log(\hat{\eta}_s)\}.$$

where  $\hat{\eta}_s = \psi_s \hat{\theta}_s$ . Let  $a_s(x_s) = \log(\hat{\theta}_s) - \log\{1 + \exp(\alpha^T x_s)(1 - \hat{\theta}_s)\}$ . Then under the logistic model

$$\begin{aligned} \eta_s &= \psi_s \hat{\theta}_s = \exp(\alpha^T x_s + \log(\hat{\theta}_s)) / \{1 + \exp(\alpha^T x_s)\} \\ &= \exp(\alpha^T x_s + a_s(x_s)) / \{1 + \exp(\alpha^T x_s + a_s(x))\} \end{aligned}$$

and  $a_s(x_s)$  has the appearance of an offset. However, it is a function of the linear predictor  $\alpha^T x_s$ . This allows an alternative iterative approach.

### 3.3. Estimating the Standard Errors

We give the asymptotic variances of our occupancy estimators in the linear logistic case. Denote the partial score function by  $Q(\boldsymbol{\alpha}, \boldsymbol{\beta}) = \partial \log(L_1(\boldsymbol{\alpha}, \boldsymbol{\beta})) / \partial \boldsymbol{\alpha}$ ,  $I(\boldsymbol{\alpha}, \boldsymbol{\beta}) = -\partial Q(\boldsymbol{\alpha}, \boldsymbol{\beta}) / \partial \boldsymbol{\alpha}^T$  and  $\tilde{B}(\boldsymbol{\alpha}, \boldsymbol{\beta}) = -\partial Q(\boldsymbol{\alpha}, \boldsymbol{\beta}) / \partial \boldsymbol{\beta}^T$ . Let  $\hat{\boldsymbol{\alpha}}(\boldsymbol{\beta})$  be the estimator of  $\boldsymbol{\alpha}$  arising from solving  $Q(\boldsymbol{\alpha}, \boldsymbol{\beta}) = 0$  for a given  $\boldsymbol{\beta}$ . We show in Appendix C that under mild regularity conditions an estimator of the variance of  $\hat{\boldsymbol{\alpha}}(\boldsymbol{\beta})$  is

$$\begin{aligned} \widehat{\text{Var}}\{\hat{\boldsymbol{\alpha}}(\hat{\boldsymbol{\beta}})\} &= \\ I\{\hat{\boldsymbol{\alpha}}(\hat{\boldsymbol{\beta}}), \hat{\boldsymbol{\beta}}\}^{-1} &+ I\{\hat{\boldsymbol{\alpha}}(\hat{\boldsymbol{\beta}}), \hat{\boldsymbol{\beta}}\}^{-1} \tilde{B}\{\hat{\boldsymbol{\alpha}}(\hat{\boldsymbol{\beta}}), \hat{\boldsymbol{\beta}}\} \hat{V}_\beta \tilde{B}\{\hat{\boldsymbol{\alpha}}(\hat{\boldsymbol{\beta}}), \hat{\boldsymbol{\beta}}\}^T I\{\hat{\boldsymbol{\alpha}}(\hat{\boldsymbol{\beta}}), \hat{\boldsymbol{\beta}}\}^{-1}. \end{aligned} \tag{7}$$

The estimated occupancy probability is  $\hat{\psi}_s = [1 + \exp\{-x_s^T \hat{\boldsymbol{\alpha}}(\hat{\boldsymbol{\beta}})\}]^{-1}$ , which is easily seen to have the estimated approximate variance  $\widehat{\text{Var}}(\hat{\psi}_s) = \{\hat{\psi}_s(1 - \hat{\psi}_s)\}^2 x_s^T \widehat{\text{Var}}\{\hat{\boldsymbol{\alpha}}(\hat{\boldsymbol{\beta}})\} x_s$ .

To compute (7) note that in both the time homogeneous and inhomogeneous cases we have

$$I(\boldsymbol{\alpha}, \boldsymbol{\beta}) = \sum_{s=1}^S x_s x_s^T \left\{ \frac{\theta_s - 2\psi_s(\boldsymbol{\alpha})\theta_s + \psi_s(\boldsymbol{\alpha})^2\theta_s^2 + w_s(1 - \theta_s)}{\{(1 - \psi_s(\boldsymbol{\alpha})\theta_s)\}^2} \right\} \psi_s(\boldsymbol{\alpha})\{1 - \psi_s(\boldsymbol{\alpha})\}. \quad (8)$$

However,  $\tilde{B}(\boldsymbol{\alpha}, \boldsymbol{\beta})$  is computed differently. In the time homogeneous case we have

$$\tilde{B}(\boldsymbol{\alpha}, \boldsymbol{\beta}) = -\frac{\sum_{s=1}^S x_s u_s^T \psi_s(1 - \psi_s)(1 - w_s)\tau(1 - \theta_s)p_s}{(1 - \psi_s\theta_s)^2}, \quad (9)$$

whereas in the time heterogeneous case we have

$$\tilde{B}(\boldsymbol{\alpha}, \boldsymbol{\beta}) = -\sum_{s=1}^S \frac{x_s \psi_s(1 - \psi_s)(1 - w_s)(1 - \theta_s) \sum_{j=1}^{\tau} p_{sj} u_{sj}^T}{(1 - \psi_s\theta_s)^2}. \quad (10)$$

Then in either case, the expression (7) holds (see Appendix C). Note that if  $p_{sj} \equiv p_s$  and  $u_{sj} \equiv u_s$  then  $\sum_{j=1}^{\tau} p_{sj} u_{sj}^T = \tau p_s u_s$  (9) and (10) are the same. In computing  $\tilde{B}(\boldsymbol{\alpha}, \boldsymbol{\beta})$  we can replace  $w_s$  by its expectation  $\psi_s\theta_s$ .

#### 4. Simulations

To evaluate the two-stage approach (described in Section 3.2) we used one site covariate for occupancy, an independent site covariate for detection and a further independent single time varying covariate that also varied between sites. These were all taken to have standard normal distributions, reflecting that it is common to standardise the covariates. We took varying parameter values to reflect different mean occupancy and detection probabilities. For each value of  $S$  and  $\tau$  we simulated the covariates once then for varying parameter values simulated occupancy and detection. We first

conducted simulations to determine which of the three methods of estimating occupancy performed best. Firstly we conducted simulations to determine which of the methods, IWLS, direct maximisation of the partial likelihood with `optim` (Partial) or iterative offset (Iterative) to use. Direct maximisation using `optim` allows different optimization methods, the option BFGS numerical maximisation method is adopted here. Comparison to CG and Nelder-Mead method displayed improved convergence for BFGS. We consider  $S = 500$  and  $\tau = 5$ ,  $\boldsymbol{\alpha} = (1, 1)$ , and  $\boldsymbol{\beta} = (-1.5, -0.5, -0.5)$  giving for our simulated covariates an average occupancy probability of 0.70 and an average probability of detection at least once at a site of 0.65. We took 1000 simulations. The results are in Table 1. Efficiencies are computed relative to the partial likelihood and are computed using the usual ratio of the variances (Efficiency) and the ratio of median absolute deviations squared (Efficiency (mad)). Median absolute deviations (mad) are given by  $\text{mad} = c \times \text{median}(|x_i - x_M|)$ , where  $c = 1/\Phi(-1)(3/4)$ ,  $\Phi(-1)(3/4)$  is the third quartile of the inverse standard normal distribution, and  $x_M$  is the median of  $x_i$ . We used the function `mad` in R to calculate these. The medians showed little bias in any of the methods although when the means were computed, direct maximisation of the partial likelihood (Partial) exhibited considerable bias. The median absolute deviations of the IWLS and Partial methods were similar as is also evident in the efficiencies computed using the mad. With a smaller number of site visits,  $\tau = 3$  in Table 2 there is now some evidence of bias in all methods and the IWLS is clearly the most efficient. In this case the average probability of detection at least once at a site was 0.47.

Next, we compare the IWLS method for the two-stage approach of es-

Table 1: Stage 2: Efficiency for estimating occupancy probabilities for the two-stage approach for three methods; IWLS, direct maximisation of the partial likelihood using `optim` (Partial), or iterative offset (Iterative). Simulation results to compare numerical methods  $S = 500$ ,  $\tau = 5$ , mean  $\psi = 0.7$ , mean  $\theta = 0.65$ ,  $\boldsymbol{\alpha} = (1, 1)$  and  $\boldsymbol{\beta} = (-1.5, -0.5, -0.5)$ .

	IWLS		Partial		Iterative	
Actual $\alpha$	1.00	1.00	1.00	1.00	1.00	1.00
Median	1.02	1.00	1.02	1.00	1.02	1.01
mad	0.25	0.25	0.25	0.26	0.32	0.31
Mean	1.03	1.02	1.97	1.47	1.15	1.15
sd	0.28	0.26	5.66	2.70	1.03	1.04
Efficiency	41656.85	10910.59			3014.89	677.40
Efficiency(mad)	100.00	107.35			61.96	67.59

timisation of occupancy to the full likelihood of MacKenzie et al. (2002). In Table 3 we consider  $S = 500$  and  $\tau = 5$ . We took 1000 simulations at each parameter combination. With a small number of standardised covariates the MacKenzie maximum likelihood estimators were expected to perform well. These were computed using the `occu` function in the R package `unmarked` (see Appendix D for a brief description). We report the median and mad of the estimates. With lower detection probabilities occasionally the IWLS algorithm did not converge in 200 iterations. In that case the partial likelihood could be directly maximised. The bias of both procedures was low. As expected the efficiencies of estimating the parameters associated with detection were low. The efficiencies of the two-stage estimator in estimating the occupancy probabilities was good and was generally around 100% for the covariate term, but less than 100% for the intercept. The large efficiencies

Table 2: Stage 2: Efficiency for estimating occupancy probabilities for the two-stage approach for three methods; IWLS, direct maximisation of the partial likelihood using `optim` (Partial), or iterative offset (Iterative). Simulation results to compare numerical methods  $S = 500$ ,  $\tau = 3$ , mean  $\psi = 0.7$ , mean  $\theta = 0.47$ ,  $\boldsymbol{\alpha} = (1, 1)$  and  $\boldsymbol{\beta} = (-1.5, -0.5, -0.5)$ .

	IWLS		Partial		Iterative	
Actual $\alpha$	1.00	1.00	1.00	1.00	1.00	1.00
Median	1.17	0.99	1.17	1.02	1.23	1.03
mad	0.57	0.24	0.62	0.31	0.68	0.54
Mean	1.17	1.05	1.34	1.15	1.81	1.67
sd	0.49	0.33	0.99	0.55	2.03	1.77
Efficiency	400.97	284.07			23.69	9.65
Efficiency(mad)	120.18	165.64			81.85	32.49

for smaller occupancy and detection probabilities were due to several unusually large maximum likelihood estimates. Similarly the small efficiencies for smaller detection probabilities but larger occupancy probabilities were due to large values of the two-stage estimates.

A plot of 1000 simulated occupancy estimates from our approach were compared to the full likelihood (see Figure 1). The model included time varying covariates using the two-stage approach for the IWLS method and the same was modelled with `occu`;  $\boldsymbol{\alpha} = (1, 1)$ ,  $\boldsymbol{\beta} = (-1.5, -0.5)$ , and  $\beta_t = -0.5$ . Overall, the two-stage estimator gave estimates that were more accurate and more consistent and that `occu` may give extreme estimates of occupancy parameters when the two-stage approach does not. There was a single outlier that was omitted from the plot for clarity. Corresponding summary statistics are given in Table 4.

Table 3: Simulation results for  $S = 500$ ,  $\tau = 5$  for four studies with mean probabilities  $(\psi, p)$ :  $(0.7, 0.65)$ ,  $(0.31, 0.65)$ ,  $(0.7, 0.37)$  and  $(0.31, 0.37)$ . Efficiency is based on the variance rather than the mad. Medians for the two-stage method (med two-stage) and full maximum likelihood estimates (med mle), as well as their median absolute deviations ‘mad two-stage’ and ‘mad mle’, respectively. Occupancy for the two-stage approach estimated with IWLS method.

	Occupancy		Detection			Occupancy		Detection		
	Int	$x_1$	Int	$x_2$	time	Int	$x_1$	Int	$x_2$	time
Mean Prob	0.70		0.65			0.31		0.65		
Actual	1.00	1.00	-1.50	-0.50	-0.50	-1.00	1.00	-1.50	-0.50	-0.50
med two-stage	1.01	1.01	-1.51	-0.51	-0.50	-0.99	1.01	-1.52	-0.50	-0.50
mad two-stage	0.26	0.23	0.11	0.10	0.07	0.19	0.18	0.16	0.15	0.11
med mle	1.01	1.01	-1.51	-0.50	-0.49	-0.99	1.01	-1.52	-0.51	-0.50
mad mle	0.25	0.23	0.09	0.07	0.07	0.18	0.18	0.14	0.11	0.10
Efficiency	90.65	101.74	66.04	52.03	93.13	93.67	99.41	69.72	54.69	91.09
Efficiency(mad)	91.64	98.57	70.62	54.81	94.00	93.19	102.40	73.01	49.57	96.52
Mean Prob	0.70		0.37			0.31		0.37		
Actual	1.00	1.00	-2.50	-0.50	-0.50	-1.00	1.00	-2.50	-0.50	-0.50
med two-stage	1.01	0.99	-2.53	-0.50	-0.50	-0.97	1.03	-2.55	-0.52	-0.50
mad two-stage	0.65	0.41	0.23	0.19	0.10	0.41	0.27	0.37	0.29	0.15
med mle	1.03	1.00	-2.51	-0.50	-0.50	-0.97	1.05	-2.53	-0.49	-0.50
mad mle	0.57	0.39	0.16	0.09	0.09	0.36	0.28	0.28	0.16	0.14
Efficiency	0.15	0.22	43.13	23.13	81.39	371.60	3223.71	50.28	23.03	81.91
Efficiency(mad)	78.85	87.63	51.67	22.50	84.41	78.39	102.95	57.02	29.27	85.60

Table 5 shows that `occu` gives estimates that are large four times more often than our approach. We present agreement between our approach and `occu` to estimating occupancy. Agreement between the two methods is defined as the number of estimates that are either both or neither greater than three ( $\hat{\alpha}_1 > 3$ ), less than or equal to three ( $\hat{\alpha}_1 \leq 3$ ), or when these disagree. `occu` gives estimates that are greater than three (i.e  $\hat{\alpha}_1 > 3$ ) four times more often than our IWLS method i.e. 36 to 12 (Table 5). The table clearly demonstrates there is no universal best method for finding estimates for occupancy. When IWLS fails i.e. does not converge, then we recommend using `optim` or `occu`.

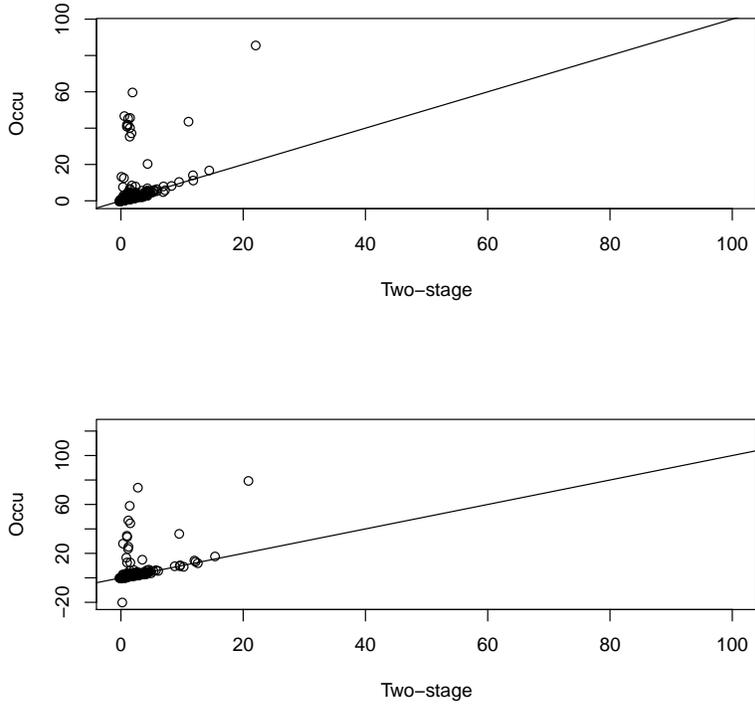


Figure 1: Comparison of estimated occupancy parameters ( $\hat{\alpha}$ ) between `occu` and two-stage method with IWLS for 1000 simulations with  $\alpha = (1, 1)$ ,  $\beta = (-1.5, -0.5)$ , and  $\beta_t = -0.5$ . Top figure shows intercept estimates and bottom figure estimates for the slope parameter.

## 5. Applications

### 5.1. Data Set 1

Hutchinson et al. (2015b) use a publicly available data set from Hutchinson et al. (2015a)<sup>3</sup> to illustrate their penalized likelihood approach. The data set contains detections of 25 avian species over 3 visits to each of 656

<sup>3</sup><https://datadryad.org//resource/doi:10.5061/dryad.t40f2>

Table 4: Simulation study of 1000 estimates of the occupancy parameters with  $\alpha = (1, 1)$ ,  $\beta = (-1.5, -0.5)$ , and  $\beta_t = -0.5$ .

	Occupancy		Detection		
	Int	$x_1$	Int	$x_2$	time
Mean Prob	0.72		0.63		
Actual	1.00	1.00	-1.50	-0.50	-0.50
med two-stage	0.98	1.03	-1.53	-0.52	-0.51
mad two-stage	0.63	0.57	0.25	0.28	0.15
sd two-stage	7.82	9.94	0.28	0.28	0.16
med mle	1.10	1.16	-1.52	-0.53	-0.51
mad mle	0.70	0.65	0.21	0.17	0.15
Efficiency	67.55	45.33	68.41	38.92	90.47
Efficiency(mad)	99.94	125.16	71.13	38.25	93.37

sites from a field study in 2011 in southern Indiana, USA. We use the entire data set. There are six site-specific vegetation covariates available (labelled `vegcov1`, `vegcov2`, `...``vegcov6`) and four time dependent survey covariates `time`, `temp`, `cloud` and `julian` measured for each visit to each site. These are included in the data data frame as `time1`, `time2`, `...``julian2`, `julian3`. All the covariates have been standardised. We consider the entire data set for the first species. We considered four models for the detection probabilities. The first only involved the site covariates, the second the site covariates and time dependent intercepts, the third site and time dependent survey covariates and the last involved site and time dependent survey covariates and time dependent intercepts. The values of the AIC from the conditional likelihood are: Site only: AIC = 1517.4, Site + Time Varying In-

Table 5: Agreement for intercept estimates greater, or less, than three when the actual value to be estimated is  $\alpha_1 = 1$ .

	occu method	
Two-stage IWLS	$\hat{\alpha}_1 \leq 3$	$\hat{\alpha}_1 > 3$
$\hat{\alpha}_1 \leq 3$	832	36
$\hat{\alpha}_1 > 3$	12	37

tercept: AIC = 1511.1, Site + Survey: AIC = 1488.3, Site + Survey + Time Varying Intercept: AIC = 1486.2. The best model of these includes the site covariates, time dependent survey covariates and time dependent intercepts. The resulting two-stage (Two-stage) estimates (with IWLS method) are displayed in Table 6 along with the full maximum likelihood estimates (Full likelihood) computed using the `occu` function in the R package `unmarked` (fitting the model with `occu` is briefly described in Appendix D). The maximum likelihood and two-stage estimates are very similar.

In the model for detection there are 6 site covariates and 4 survey covariates. This gives  $2^{10} = 1024$  possible models (or  $2^{11}$  if one allows time varying intercepts.) Whilst this is a large number of models, in the absence of variable selection methods in `VGAM` it is nevertheless feasible to compute the AIC for each model. We can then repeat this process for the model for occupancy after fixing the best detection model. The best fitting model for the detection probabilities using the AIC is indicated in Table 6. The function `vglm` allows more flexibility in the modelling. For example, by changing `parallel.t=FALSE~0` to `parallel.t=TRUE~0` the coefficients associated with each variable in the detection model may be time varying. We do not pursue this further here. Of course as occupancy is assumed constant over

the visits we do not model the occupancy coefficients as time varying.

Table 6: Occupancy and detection estimates for full likelihood and two-stage approaches for the detection model with site and survey covariates and time varying intercept for the Hutchinson data (\* indicates the variables retained in the best fitting model using the two-stage approach). For each covariate, we report its: estimate (Estimate), standard error (se), Student's  $t$ -statistic ( $t$ ), and  $p$ -value ( $p$ ).

Parameter	Full Likelihood				Two-stage			
	Estimate	se	$t$	$p$	Estimate	se	$t$	$p$
Occupancy $\psi$								
Intercept*	2.27	0.15	14.98	0.00	2.26	0.15	14.91	0.00
vegcov1*	0.50	0.18	2.78	0.01	0.52	0.17	3.00	0.00
vegcov2	0.03	0.17	0.15	0.88	0.01	0.17	0.04	0.97
vegcov3	0.07	0.17	0.41	0.68	0.06	0.16	0.34	0.73
vegcov4*	0.37	0.13	2.89	0.00	0.37	0.12	3.03	0.00
vegcov5	0.14	0.13	1.06	0.29	0.14	0.13	1.10	0.27
vegcov6*	-0.29	0.16	-1.85	0.06	-0.29	0.15	-1.88	0.06
Detection $p$								
Intercept:1*	1.07	0.30	3.60	0.00	1.09	0.30	3.67	0.00
Intercept:2*	1.48	0.12	12.00	0.00	1.48	0.12	12.04	0.00
Intercept:3*	2.27	0.30	7.70	0.00	2.26	0.30	7.62	0.00
vegcov1*	0.56	0.09	6.06	0.00	0.55	0.09	6.02	0.00
vegcov2*	-0.25	0.09	-2.79	0.01	-0.25	0.09	-2.76	0.01
vegcov3	-0.10	0.09	-1.16	0.24	-0.09	0.09	-1.05	0.30
vegcov4*	0.18	0.08	2.37	0.02	0.18	0.07	2.34	0.02
vegcov5*	0.10	0.08	1.34	0.18	0.11	0.07	1.46	0.14
vegcov6*	-0.10	0.09	-1.18	0.24	-0.11	0.09	-1.27	0.20
time	-0.07	0.07	-0.93	0.35	-0.07	0.07	-0.98	0.33
temp*	-0.24	0.08	-3.09	0.00	-0.24	0.08	-3.11	0.00
cloud*	-0.13	0.07	-1.90	0.06	-0.13	0.07	-1.93	0.05
julian*	-0.74	0.23	-3.23	0.00	-0.73	0.23	-3.18	0.00

## 5.2. Data II

A smaller data set is given on the website James Peterson <sup>4</sup> that presents data on detections of brook trout collected via electrofishing in three 50 m sections of streams at 57 sites in the Upper Chattahoochee 371 River basin,

<sup>4</sup>[http://people.oregonstate.edu/~peterjam/occupancy\\_workshop/hands\\_on.html](http://people.oregonstate.edu/~peterjam/occupancy_workshop/hands_on.html)

USA. These data contained a site covariate, Elevation (Ele) and a time dependent covariate stream mean cross-sectional area (CSA). These variables are on quite different scales. The average elevation was approximately 2861 and the mean cross-sectional area was less than 2. We considered four models, just the site covariates, site covariates and time varying intercepts, site and survey covariates and site and survey covariates with time varying intercepts. Using the default settings in `occu` the estimates did not converge. This was rectified by using the “Nelder-Mead” method set to a maximum of 2000 iterations. The two-stage estimator had no such problems. The estimates for the unstandardised data are in Table 7 (a). The estimates are generally similar. For the standardised data, `occu` with the default options did converge. The results are given in Table 7 (b). The estimates are again quite similar.

Table 7: Occupancy and detection estimates for full likelihood and two-stage approaches for the (a) unstandardised and (b) standardised brook trout data. For each covariate, we report its: estimate (Estimate), standard error (se), Student's  $t$ -statistic ( $t$ ), and  $p$ -value ( $p$ ). Occupancy for the two-stage approach estimated with IWLS method.

Parameter	Full Likelihood				Two-stage			
	Estimate	se	$t$	$p$	Estimate	se	$t$	$p$
(a) Unstandardised								
Occupancy $\psi$								
Intercept	-3.9716	0.6858	-5.7914	0.0000	-4.0452	1.1218	-3.6060	0.0003
Ele	0.0013	0.0003	4.5338	0.0000	0.0013	0.0004	3.6441	0.0003
Detection $p$								
Intercept	0.0580	0.7352	0.0788	0.9372	-0.1609	1.2397	-0.1298	0.8968
Ele	0.0004	0.0002	1.9697	0.0489	0.0004	0.0003	1.2516	0.2107
CSA	-0.8325	0.2822	-2.9503	0.0032	-0.7438	0.2873	-2.5888	0.0096
(b) Standardised								
Occupancy $\psi$								
Intercept	-0.19	0.36	-0.52	0.60	-0.34	0.32	-1.04	0.30
Ele	1.53	0.45	3.42	0.00	1.48	0.40	3.71	0.00
Detection $p$								
Intercept	-0.14	0.35	-0.38	0.70	-0.16	0.36	-0.44	0.66
Ele	0.36	0.35	1.04	0.30	0.43	0.37	1.18	0.24
CSA	-0.82	0.28	-2.97	0.00	-0.80	0.28	-2.81	0.00

## 6. Discussion

In Karavarsamis and Huggins (2017) we examined the two-stage approach for the homogeneous occupancy model. Here we examined the two-stage approach for the heterogeneous occupancy model where the occupancy and detection probabilities now depend on covariates that may vary between sites and over time.

In our applications here the two-stage estimator gave similar estimates to the full maximum likelihood with the `occu` function in package `unmarked`. For the large standardised data set first considered the estimates from the two methods were very similar. The two-stage method has advantages in model selection as the dimension of the space to be searched can be enormously reduced. By considering two smaller dimensional parameter spaces and using IWLS in both stages it is also numerically more stable so that standardisation is less important. It also gives access to the `VGAM` methodology in estimating detection. We defer further exploration elsewhere.

The default in the `occu` function in the `unmarked` package uses a vector of zeroes as starting values and if the algorithm does not converge suggests the user provides starting values. However, there is no guidance on how to find suitable values. A simulation study showed that `occu` may give extreme estimates of occupancy parameters when the two-stage does not.

If there are too few redetections the two-stage estimator can fail. This results from conditioning on at least one detection. However, when the main focus is on estimating occupancy, the occupancy probability appears to be relatively insensitive for small changes in detection probability (Karavarsamis and Huggins, 2017).

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## **Appendix A. Conditional Likelihood using VGAM**

The R package `VGAM` (Yee, 2010) is a powerful and flexible package that fits models to vector responses. As such, at first glance it can be overwhelming.

However, its handling of time dependent covariates makes it preferable to writing one's own functions. Here we give a description of how it can be used to fit some common models to detections using conditional likelihood in the first stage of our approach.

*Appendix A.1. Fitting Time Independent Covariates for Detection*

In our two-stage approach the conditional likelihood fits the model for detection to data from the sites where there was at least one detection. This can be done the `posbinomial` family in the VGAM function `vglm`. Firstly the data is reduced to those sites where there was at least one detection. When there is no time dependence, computing the estimates using `vglm` is straightforward. We illustrate this for the data of Hutchinson et al. (2015b,a) as these data contain both site and visit (i.e. time dependent) covariates. For these data, the data frame `data` is a reduced data frame that contains data from the sites where occupancy was detected. The variable  $Y$  is the number of times the species was detected at each occupied site,  $\tau$  is the number of visits to each site, and site covariates are `vegcov1, vegcov2, . . . , vegcov6`. See Figure A.2 for selected output ( $\tau = 3$  in this example). The parameter estimates may then be used in the second stage of the analysis.

With the univariate response  $Y$ , the implementation is very similar to `glm`. The term `omit.constant=TRUE` does not affect the fitting but removes the constant terms from the computation of the AIC. These estimates may then be input into the second stage procedure to estimate parameters associated with the occupancy model.

```

> V.out=vglm(cbind(Y,3-Y)~vegcov1+vegcov2+vegcov3+vegcov4
             +vegcov5+vegcov6,
             family=posbinomial(omit.constant=TRUE),data=data)
> coef(V.out)
# (Intercept)      vegcov1      vegcov2      vegcov3      vegcov4
#  1.5590909    0.5493825   -0.2512287   -0.1048756    0.1656597
#  vegcov5      vegcov6
#  0.1186192   -0.1277806

```

Figure A.2: Fitting the detection model for time homogeneous covariates.

### *Appendix A.2. Fitting Time Dependent Covariates for Detection*

Time dependent models for detection may be fitted to data using the `posbernoulli.t` family in the `vglm` function in `VGAM`. Fitting these models is more complex as many more models are available and the response consists of the detections on each visit to the site and is hence multivariate. We again use the data from Hutchinson et al. (2015b,a). The time dependent covariates are time, temp, cloud and julian measured for each visit to each site. These are included in the data data frame as `time1`, `time2`, `...`, `julian2`, `julian3`. With a vector valued response there is the possibility that the coefficient associated with a covariate may change with the visit, so the associated modelling and hence the functions to fit the models are more complex. See Yee (2010, §6.3) for a worked example in a capture-recapture context. In Figure A.3 we first fit a simple model with time dependent intercepts and the relationship with the site covariates remains independent of time. This was specified through the `parallel.t` argument to the `posbernoulli.t` family. Note that

```

> V.out=vglm(cbind(survey1,survey2,survey3)
             ~ vegcov1+vegcov2+vegcov3+vegcov4+vegcov5+vegcov6,
             family=posbernoulli.t(parallel.t=FALSE~1), data=data)
> coef(V.out)
# (Intercept):1 (Intercept):2 (Intercept):3 vegcov1 vegcov2
# 1.8583766 1.5130892 1.3527893 0.5515551 -0.2522520
# vegcov3 vegcov4 vegcov5 vegcov6
# -0.1052631 0.1663444 0.1190595 -0.1282785

```

Figure A.3: Fitting a model with time dependent intercepts.

`parallel.t=FALSE~1` is the default for the `posbernoulli.t` family but for clarity we explicitly incorporate it in Figure A.3.

Incorporating time dependent covariates is a little more complex and requires use of the `xij` and `form2` arguments in `VGAM`. The `form2` argument is straightforward. It gives all the variables in the model and needs to be included if `xij` is used. The `xij` argument specifies that covariates have different values at different visits. To implement it is necessary to construct a new variable, for example `time.tij`, for each time dependent variable in the model and incorporate them in the data frame. In our case this gives four new variables, `time.tij`, `temp.tij`, `cloud.tij` and `julian.tij` in Figure A.4.

## Appendix B. Iterative Weighted Least Squares

The potential instability of the maximum likelihood estimates when computed using numerical optimization, through the function `optim` in R mo-

```

> V.out=vglm(cbind(survey1,survey2,survey3)
~vegcov1+vegcov2+vegcov3+vegcov4
+vegcov5+vegcov6+time.tij+temp.tij+cloud.tij+julian.tij,
data=Data.all,
xij=list(time.tij~time1+time2+time3-1,temp.tij~temp1+temp2+temp3-1,
cloud.tij~cloud1+cloud2+cloud3-1,julian.tij~julian1+julian2
+julian3-1),
family=posbernoulli.t(parallel.t=FALSE~0),
form2=~vegcov1+vegcov2+vegcov3+vegcov4+vegcov5+vegcov6+time.tij
+temp.tij+cloud.tij+julian.tij+time1+time2+time3+temp1+temp2
+temp3+cloud1+cloud2+cloud3+julian1+julian2+julian3)
> coef(V.out)
# (Intercept)  vegcov1    vegcov2    vegcov3    vegcov4
# 1.60651791  0.54525171 -0.24061702 -0.08727207  0.16955603
# vegcov5  vegcov6   time.tij  temp.tij  cloud.tij  julian.tij
# 0.108527 -0.112085 -0.069456 -0.238605 -0.161028 -0.264658

```

Figure A.4: Fitting a model using with time varying covariates but constant intercept for the two-stage approach in vglm.

tivated us to develop an iterative weighted least squares (IWLS) approach. This is quite straightforward for the logistic model in our two-stage approach.

Recall  $E(w_s) = \eta_s = \theta_s \psi_s$ . Let  $\boldsymbol{\eta} = (\eta_1, \dots, \eta_S)^T$ ,  $\boldsymbol{w} = (w_1, \dots, w_S)^T$  and the  $q_0 \times S$  matrix  $X$  has sth column  $x_s$ . Then, as  $\theta_s$  is not a function of  $\boldsymbol{\alpha}$ , maximising the partial log-likelihood (6) is equivalent to maximising  $\ell(\boldsymbol{\eta}) = \sum_{s=1}^S \{(1 - w_s) \log(1 - \eta_s) + w_s \log(\eta_s)\}$ . Then, with  $V = \text{diag}\{(1 - \boldsymbol{\eta})\boldsymbol{\eta}\}$  we have  $\boldsymbol{u}(\boldsymbol{\eta}) = \partial \ell(\boldsymbol{\eta}) / \partial \boldsymbol{\eta} = V^{-1}(\boldsymbol{w} - \boldsymbol{\eta})$ . Let  $\gamma_s = \boldsymbol{x}_s^T \boldsymbol{\alpha}$  and  $\boldsymbol{\gamma} = (\gamma_1, \dots, \gamma_S) = X\boldsymbol{\alpha}$ . Now,  $\partial \eta_s / \partial \gamma_s = \theta_s \psi_s (1 - \psi_s)$  and  $\partial \gamma_s / \partial \boldsymbol{\alpha} = \boldsymbol{x}_s$  so that  $\partial \eta_s / \partial \boldsymbol{\alpha} = \theta_s \psi_s (1 - \psi_s) \boldsymbol{x}_s$ . That is,  $\partial \boldsymbol{\eta}^T / \partial \boldsymbol{\alpha} = XU$  where  $U = \text{diag}\{\theta_s \psi_s (1 - \psi_s)\}$  or the partial score equations may be written as  $\boldsymbol{u}(\boldsymbol{\alpha}) = (\partial \boldsymbol{\eta}^T / \partial \boldsymbol{\alpha}) \boldsymbol{u}(\boldsymbol{\eta}) = XUV^{-1}(\boldsymbol{w} - \boldsymbol{\eta}(\boldsymbol{\alpha}))$ . The expected conditional Fisher information is then  $J(\boldsymbol{\alpha}) = -E(\partial \boldsymbol{u}(\boldsymbol{\alpha}) / \partial \boldsymbol{\alpha}^T) = XUV^{-1}UX^T$ . Recall  $\boldsymbol{Z} = UX\boldsymbol{\alpha}^{(k)} + \boldsymbol{w} - \boldsymbol{\eta}(\boldsymbol{\alpha}^{(k)})$ . Then

$$\begin{aligned} \boldsymbol{\alpha}^{(k+1)} &\approx \boldsymbol{\alpha}^{(k)} + J(\boldsymbol{\alpha})^{-1} \boldsymbol{u}(\boldsymbol{\alpha}^{(k)}) \\ &= \boldsymbol{\alpha}^{(k)} + (XUV^{-1}UX^T)^{-1} XUV^{-1}(\boldsymbol{w} - \boldsymbol{\eta}(\boldsymbol{\alpha}^{(k)})) \\ &= (XUV^{-1}UX^T)^{-1} XUV^{-1} (UX\boldsymbol{\alpha}^{(k)} + \boldsymbol{w} - \boldsymbol{\eta}(\boldsymbol{\alpha}^{(k)})) \\ &= (XUV^{-1}UX^T)^{-1} XUV^{-1} \boldsymbol{Z}. \end{aligned}$$

This gives the iterative procedure of Section 3.2.1.

### Appendix C. Derivation of the Standard Errors

We outline the proof of (7) for the linear model with logistic link. Let  $\boldsymbol{\alpha}_0$  and  $\boldsymbol{\beta}_0$  denote the true values of  $\boldsymbol{\alpha}$  and  $\boldsymbol{\beta}$  and let  $\widehat{\boldsymbol{\beta}}$  be a consistent estimator of  $\boldsymbol{\beta}$ . Here this will be the conditional likelihood estimator of  $\boldsymbol{\beta}$  but our results are more general than that. We suppose that for a  $q_o \times q_p$  matrix

$B(\boldsymbol{\alpha}, \boldsymbol{\beta})$ , and a  $q_o \times q_o$  matrix  $A(\boldsymbol{\alpha}, \boldsymbol{\beta})$ ,

$$\begin{aligned} S^{-1} \tilde{B}(\boldsymbol{\alpha}_0, \boldsymbol{\beta}_0) &= S^{-1} \frac{\partial Q(\boldsymbol{\alpha}_0, \boldsymbol{\beta}_0)}{\partial \boldsymbol{\beta}_0^T} \rightarrow B(\boldsymbol{\alpha}_0, \boldsymbol{\beta}_0), \\ -S^{-1} \frac{\partial Q(\boldsymbol{\alpha}_0, \boldsymbol{\beta}_0)}{\partial \boldsymbol{\alpha}_0^T} &\rightarrow A(\boldsymbol{\alpha}_0, \boldsymbol{\beta}_0) \end{aligned}$$

and that the central limit theorem is applicable so that

$$S^{-1/2} Q(\boldsymbol{\alpha}_0, \boldsymbol{\beta}_0) \xrightarrow{d} N(0, \Sigma_Q). \quad (\text{C.1})$$

We also suppose that the estimators  $\hat{\boldsymbol{\beta}}$  arising from the first stage are consistent and satisfy  $S^{1/2}(\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0) \xrightarrow{d} N(0, \Sigma_\beta)$  for some  $q \times q$  matrix  $\Sigma_\beta$ . That is,  $\text{Var}(\hat{\boldsymbol{\beta}}) = \Sigma_\beta/S$ . Note that using `vglm` to estimate  $\boldsymbol{\beta}$  using conditional likelihood yields an estimate of  $\text{Var}(\hat{\boldsymbol{\beta}}|O)$ . Then we approximate  $\Sigma_\beta$  by  $S\text{Var}(\hat{\boldsymbol{\beta}}|O)$ . Finally, we suppose that the partial score functions for  $\boldsymbol{\alpha}$  are uncorrelated with those for  $\boldsymbol{\beta}$ . We have noted in §3 that this holds for the likelihood conditional on at least one detection at a site.

The log-partial likelihood is

$$\begin{aligned} \ell(\boldsymbol{\alpha}, \boldsymbol{\beta}) &= \sum_{s=1}^S \{(1 - w_s) \log(1 - \psi_s(\boldsymbol{\alpha})\theta_s) + w_s \log(\psi_s(\boldsymbol{\alpha}))\}, \text{ so that} \\ Q(\boldsymbol{\alpha}, \boldsymbol{\beta}) &= \partial \ell(\boldsymbol{\alpha}, \boldsymbol{\beta}) / \partial \boldsymbol{\alpha} = \sum_{s=1}^S x_s \{w_s - \psi_s(\boldsymbol{\alpha})\theta_s\} (1 - \psi_s(\boldsymbol{\alpha})) / \{1 - \psi_s(\boldsymbol{\alpha})\theta_s\}. \end{aligned}$$

The first order expansion of  $Q(\hat{\boldsymbol{\alpha}}, \hat{\boldsymbol{\beta}})$  about  $\boldsymbol{\alpha}_0$  yields

$$S^{1/2} \left( \hat{\boldsymbol{\alpha}}(\hat{\boldsymbol{\beta}}) - \boldsymbol{\alpha}_0 \right) = \left\{ S^{-1} I(\boldsymbol{\alpha}_0, \hat{\boldsymbol{\beta}}) \right\}^{-1} S^{-1/2} Q(\boldsymbol{\alpha}_0, \hat{\boldsymbol{\beta}}),$$

and that of  $Q(\boldsymbol{\alpha}_0; \hat{\boldsymbol{\beta}})$  about  $\boldsymbol{\beta}_0$  yields

$$S^{-1/2} Q(\boldsymbol{\alpha}_0; \hat{\boldsymbol{\beta}}) \approx S^{-1/2} Q(\boldsymbol{\alpha}_0, \boldsymbol{\beta}_0) + S^{-1} \tilde{B}(\boldsymbol{\alpha}_0, \boldsymbol{\beta}_0) S^{1/2} (\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0)$$

which together give

$$S^{1/2} (\hat{\boldsymbol{\alpha}}(\hat{\boldsymbol{\beta}}) - \boldsymbol{\alpha}_0) \approx A(\boldsymbol{\alpha}_0, \boldsymbol{\beta})^{-1} \left\{ S^{-1/2} Q(\boldsymbol{\alpha}_0, \boldsymbol{\beta}_0) + B(\boldsymbol{\alpha}, \boldsymbol{\beta}_0) S^{1/2} (\hat{\boldsymbol{\beta}} - \boldsymbol{\beta}_0) \right\}.$$

The central limit theorem and recalling that the partial score functions are uncorrelated then gives

$$S^{1/2}(\widehat{\boldsymbol{\alpha}}(\widehat{\boldsymbol{\beta}}) - \boldsymbol{\alpha}_0) \sim N_p \left( 0, A(\boldsymbol{\alpha}_0, \boldsymbol{\beta}_0)^{-1} \left\{ \Sigma_Q + B(\boldsymbol{\alpha}_0, \boldsymbol{\beta}_0) \Sigma_{\boldsymbol{\beta}} B(\boldsymbol{\alpha}_0, \boldsymbol{\beta}_0)^T \right\} A(\boldsymbol{\alpha}_0, \boldsymbol{\beta}_0)^{-T} \right),$$

where

$$\Sigma_Q = S^{-1} \text{Var}(Q(\boldsymbol{\alpha}_0, \boldsymbol{\beta}_0)) = S^{-1} E(I(\boldsymbol{\alpha}_0, \boldsymbol{\beta}_0)).$$

That is  $\text{Var}\{\widehat{\boldsymbol{\alpha}}(\widehat{\boldsymbol{\beta}})\} = S^{-1} \{A(\boldsymbol{\alpha}_0, \boldsymbol{\beta}_0)^{-1} + A(\boldsymbol{\alpha}_0, \boldsymbol{\beta}_0)^{-1} B(\boldsymbol{\alpha}_0, \boldsymbol{\beta}_0) \Sigma_{\boldsymbol{\beta}} B(\boldsymbol{\alpha}_0, \boldsymbol{\beta}_0)^T A(\boldsymbol{\alpha}_0, \boldsymbol{\beta}_0)^{-T}\}$ .

To estimate the standard errors, recall  $I(\boldsymbol{\alpha}, \boldsymbol{\beta}) = -\partial Q(\boldsymbol{\alpha}, \boldsymbol{\beta})/\partial \boldsymbol{\alpha}^T$  yielding

(8).

Next we determine  $\widetilde{B}(\boldsymbol{\alpha}, \boldsymbol{\beta})$  in the time homogeneous case. As

$$\frac{\partial Q(\boldsymbol{\alpha}, \boldsymbol{\beta})}{\partial \theta_s} = -\frac{x_s \psi_s (1 - \psi_s) (1 - w_s)}{(1 - \psi_s \theta_s)^2}, \quad (\text{C.2})$$

and  $\theta_s = 1 - (1 - p_s)^\tau$ , the chain rule gives,

$$q_s = \frac{\partial Q(\boldsymbol{\alpha}, \boldsymbol{\beta})}{\partial p_s} = -\frac{x_s \psi_s (1 - \psi_s) (1 - w_s) \tau (1 - p_s)^{\tau-1}}{(1 - \psi_s \theta_s)^2}.$$

As  $\partial p_s / \partial \beta = p_s (1 - p_s) u_s$  we then see that

$$\frac{\partial Q(\boldsymbol{\alpha}, \boldsymbol{\beta})}{\partial \boldsymbol{\beta}^T} = \widetilde{B}(\boldsymbol{\alpha}, \boldsymbol{\beta}) = -\sum_{s=1}^S \frac{x_s u_s^T \psi_s (1 - \psi_s) (1 - w_s) \tau (1 - p_s)^\tau p_s}{(1 - \psi_s \theta_s)^2}.$$

As  $\Sigma_{\boldsymbol{\beta}} = S \text{Var}(\widehat{\boldsymbol{\beta}}) = S V_{\boldsymbol{\beta}}$  where  $V_{\boldsymbol{\beta}}$  is the covariance matrix of  $\widehat{\boldsymbol{\beta}}$  and it is easily seen that  $\text{Var}\{\widehat{\boldsymbol{\alpha}}(\widehat{\boldsymbol{\beta}})\}$  reduces to (7).

In the time heterogeneous case  $\theta_s = 1 - \prod_{j=1}^{\tau} (1 - p_{sj})$ . Hence for the logistic model,

$$\frac{\partial \theta_s}{\partial \beta} = \sum_{j=1}^{\tau} \prod_{k \neq j} (1 - p_{sk}) \frac{\partial p_{sj}}{\partial \beta} = \sum_{j=1}^{\tau} \prod_{k=1}^{\tau} (1 - p_{sk}) p_{sj} u_{sj} = (1 - \theta_s) \sum_{j=1}^{\tau} p_{sj} u_{sj}.$$

As (C.2) still holds this yields the modification of the expression (7) for the standard errors as given in §3.1.2.

## Appendix D. Fitting the Full Likelihood with `occu`

The use of `occu` is well documented. Here, we briefly describe its use as it handles time varying (or time dependent) covariates differently to `vglm`. To fit our full model using `occu` we first construct a matrix of factors, `Visit`, corresponding to the three visits. We then construct a list `Obs` that contains data frames of the time varying covariates. This is then converted into an `unmarkedFrameOccu` object, `D`. The model is then fitted to the data, as shown in Figure D.5. Thus in either the `vglm` or `occu` approaches there is an initial data manipulation step requiring construction of an appropriately structured data frame, then the fitting to data. With `vglm` there is then a second step to estimate the occupancy model.

```

> Visit=matrix(as.factor(c(rep("a",656),rep("b",656),rep("c",656))),
  ncol=3)
> Obs=list(time=as.data.frame(Model.out@T.ij[,c(1,5,9)]),
  temp=as.data.frame(Model.out@T.ij[,c(2,6,10)]),
  cloud=as.data.frame(Model.out@T.ij[,c(3,7,11)]),
  julian=as.data.frame(Model.out@T.ij[,c(4,8,12)]),
  Visit=as.data.frame(Visit))
> D=unmarkedFrameOccu(y=Model.out@Detect,
  siteCovs=as.data.frame(Model.out@X[,-1]),obsCovs=Obs)
> 0.5.out=occu(~Visit+vegcov1+vegcov2+vegcov3+vegcov4+vegcov5+vegcov6
  +time+temp+cloud+julian-1~vegcov1+vegcov2+vegcov3+vegcov4+vegcov5
  +vegcov6,data=D,engine=c("C"))
> 0.5.out@estimates

```

Figure D.5: Fitting a model with occu for time varying covariates on the full model.