COM-Poisson models with varying dispersion

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1 Introduction

Standard Gaussian linear models are based on the assumption of variance homogeneity (Aitkin 1987). Generalized linear models relax this assumption by assuming the observations come from some distribution in the exponential family (Nelder & Wedderburn 1972). A key feature of exponential family distribution is the so-called mean-variance relationship, i.e. the variance is a deterministic function of the mean, $\text{Var}(Y) = \phi V(\mu)$. The main examples are $V(\mu) = \mu(1-\mu)$ for the binomial distribution, $V(\mu) = \mu$ for the Poisson distribution, $V(\mu) = \mu^2$ for the gamma distribution, and $V(\mu) = \mu^3$ for the inverse-Gaussian distribution (McCullagh & Nelder 1989). This allows modelling specific heterogeneity by assuming an appropriate distribution. However, once the mean-variance relationship is specified, the variance is assumed to be known up to a constant of proportionality, the dispersion parameter ϕ. To provide more flexibility in the analysis of heterogeneous count data, we explore methods for modelling dispersion as a function of covariates.

Modelling dispersion with covariates in the analysis of count data has received little attention in the literature. The class of double generalized linear models (Smyth 1988, McCullagh & Nelder 1989, Smyth & Verbyla 1999) provide a possible approach. This class has been widely explored for continuous data. Smyth (1988) discussed this using a double generalized linear model based on the gamma distribution. An adjusted likelihood method for estimation and inference was presented by Smyth & Verbyla (1999). Paula (2013) discussed diagnostics for this class and used gamma distributed data as an illustration. Andersen & Bonat (2017) extended the double generalized linear model by considering compound Poisson distributions. In the discrete data context, Vieira et al. (2011) proposed a Bayesian analysis using double generalized linear models for binomial data.

Another approach that has gained momentum in the last decade is the generalized additive models for location, shape, and scale (GAMLSS) (Rigby & Stasinopoulos 2005). This approach extends the generalized linear models in different directions: (i) the distribution for the response variable can be selected from a more general family; the only restriction is that the derivatives with respect to each parameter must be computable, (ii) up to four parameters of the distribution can depend on covariates, and (iii) the systematic relationship between covariates and parameters can be parametric (linear predictor) or nonparametric (smooth) functions.

In this paper, we propose to jointly model the mean and dispersion based on the COM-Poisson distribution. This approach is very similar to that of GAMLSS, however, we develop and explore our own estimation methods. This approach allows modelling of data that exhibit both under- and overdispersion, depending upon the experimental conditions.

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2 Motivating data sets

2.1 Toxicity of nitrofen in aquatic systems

Nitrofen is a herbicide that was used extensively for the control of broad-leaved and grass weeds in cereals and rice. Although it is relatively non-toxic to adult mammals, nitrofen is a significant tetragen and mutagen. It is also acutely toxic to cladoceran zooplankton, including being reproductively toxic. Nitrofen is no longer in commercial use in the United States, having been the first pesticide to be withdrawn due to tetragenic effects (Bailer & Oris 1994).

This data set comes from an experiment to measure the reproductive toxicity of the herbicide nitrofen on a species of zooplankton (*Ceriodaphnia dubia*). Fifty animals were randomized into batches of ten and each batch was placed in a solution with a measured concentration of nitrofen ($0, 0.8, 1.6, 2.35$ and 3.10 μg/10^2litre) (`dose`). Subsequently, the number of live offspring was recorded.

Figure 1 shows the data and summary statistics for each batch. It is clear that the number of live offspring decreases as the nitrofen dose increases. However, it seems that the dispersion is also influenced by the nitrofen concentration level, with underdispersion for low doses and overdispersion for high doses.

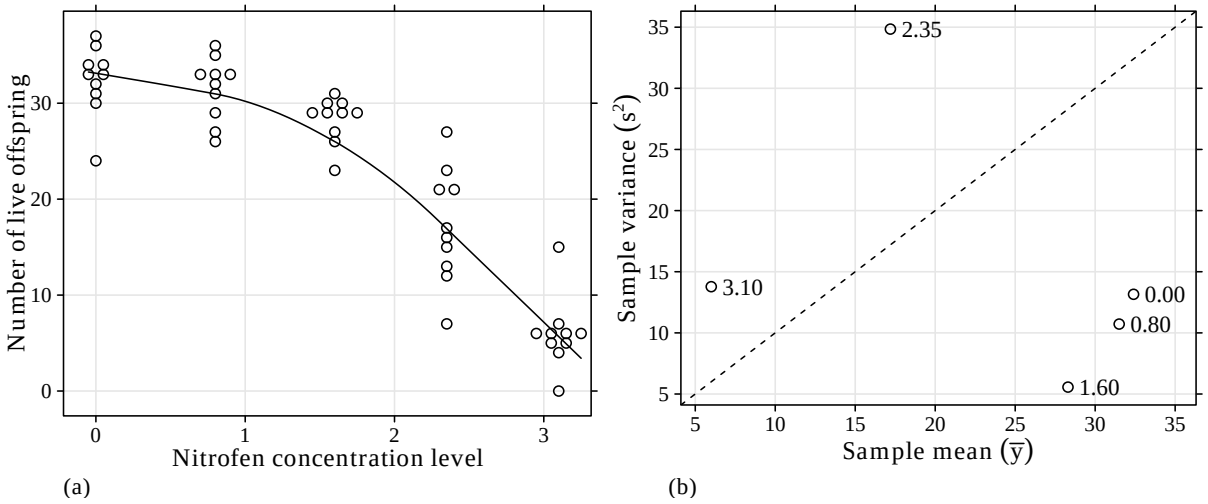

Figure 1: (a) Number of live offspring observed for each nitrofen concentration level (solid lines represent loess curve) and (b) sample variance against sample mean for each concentration level (dotted line is the identity line).

2.2 Effect of Soil moisture and potassium fertilizer on soybean culture

Tropical soils are usually poor in potassium (K) and when cultivated with soybean require potassium fertilizer to give satisfactory yields. Soybean production is also affected by prolonged exposure to water deficit. As potassium is a nutrient involved in the water balance of the plant, it is hypothesized that a good supply of potassium helps to avoid reduced productivity.

To evaluate the effects of potassium and soil humidity levels on soybean production Serafim et al. (2012) conducted a 5×3 factorial experiment in a randomized complete block design with 5 replicates. Five different potassium doses (0, 0.3, 0.6, 1.2 and $1.8 \times 100\text{mg dm}^{-3}$) were applied to the soil and soil moisture levels were controlled at (37.5, 50, and 62.5%) . The experiment was carried out in a greenhouse and the experimental units were pots with two plants in each. The count response measured was the total number of pods per pot.

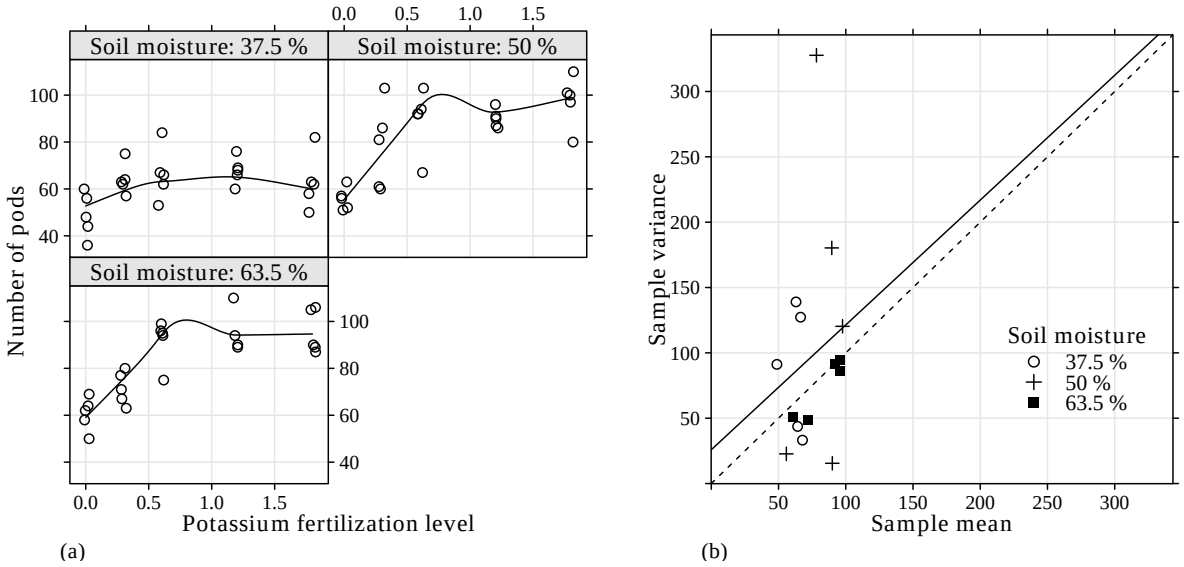

Figure 2: (a) Number of pods observed for each potassium fertilization dose and soil moisture level (solid lines represent loess curve) and (b) sample variance against sample mean for each soil moisture level (dotted line is the identity line and solid line is the least-square line).

Figure 2 shows the data and summary statistics for each batch. The smoothers in Figure 2(a) indicate a quadratic, or threshold, effect of the potassium levels. In Figure 2(b), the plot of samples variances against sample means indicates over- and under-dispersion, with the dispersion possibly different for each soil moisture level.

3 COM-Poisson models with varying dispersion

The COM-Poisson distribution is a two-parameter generalization of the Poisson distribution that can handle under-, over- and equidispersion (Shmueli et al. 2005, Sellers & Shmueli 2010). The probability mass function of the COM-Poisson distribution is given by

$$\Pr(Y = y) = \frac{\lambda^y}{(y!)^\nu \mathrm{Z}(\lambda, \nu)}, \quad \text{where} \quad \mathrm{Z}(\lambda, \nu) = \sum_{j=0}^{\infty} \frac{\lambda^j}{(j!)^\nu}, \quad \text{with} \quad y = 0, 1, 2, \ldots. \tag{1}$$

The $\mathrm{Z}(\lambda, \nu)$ is a normalizing constant that cannot be expressed in closed form, except for special cases.

The moments for the COM-Poisson distribution also cannot be obtained in closed forms. Shmueli et al. (2005) showed that the expectation of the COM-Poisson distribution

can be approximated by

$$\mathrm{E}(Y) = \frac{\mathrm{d}\{\log[\mathrm{Z}(\lambda,\nu)]\}}{\mathrm{d}\lambda} \approx \lambda^{1/\nu} - \frac{\nu-1}{2\nu}.$$

The parameter ν is the dispersion parameter and has a clear interpretation. When $\nu = 1$, the Poisson distribution results as a special (equidispersion) case, while for $0 < \nu < 1$ we have overdispersion and for $\nu > 1$ underdispersion. On the other hand, the parameter λ has no clear interpretation, except for $\nu = 1$ when it is a rate parameter and the Poisson mean, and in general it is strongly related to ν. To circumvent this dependency, Ribeiro Jr et al. (2018) propose a reparameterization of the COM-Poisson distribution to provide an (approximate) mean parameter. Replacing λ by the new parameter $\mu > 0$,

$$\mu = \lambda^{1/\nu} - \frac{\nu-1}{2\nu} \quad \Rightarrow \quad \lambda = \left(\mu + \frac{(\nu-1)}{2\nu}\right)^{\nu},$$

the authors showed that the new parameterization has good properties for estimation and inference, with approximate orthogonality of λ and ν. They proposed the use of a regression model for this approximate mean, rather than for λ as in Sellers & Shmueli (2010), and here we extend this to allow both μ and ν to depend on covariates.

Let y_i, $i = 1, 2, \ldots, n$ be a set of independent realizations of Y_i following a COM-Poisson distribution with parameters μ_i and ν_i. The proposed COM-Poisson varying dispersion model assumes

$$\eta_i = g(\mu_i) = \boldsymbol{x}_i^\top \boldsymbol{\beta} \quad \text{and} \quad \xi_i = h(\nu_i) = \boldsymbol{z}_i^\top \boldsymbol{\gamma},$$

where $\boldsymbol{\beta} = (\beta_1, \beta_2, \ldots, \beta_p)^\top$ and $\boldsymbol{\gamma} = (\gamma_1, \gamma_2, \ldots, \gamma_q)^\top$ are the parameters to be estimated, $\boldsymbol{x}_i = (x_{i1}, x_{i2}, \ldots, x_{np})^\top$ and $\boldsymbol{z}_i = (z_{i1}, z_{i2}, \ldots, z_{nq})^\top$ are vectors of known covariates, and $g(.)$ and $h(.)$ are suitable link functions. Here, we use the logarithmic link function for both mean and dispersion to avoid any range constraints.

The COM-Poisson model with varying dispersion is quite similar to the double generalized linear model approach, both extend generalized linear models to include the dispersion as well as the mean. However, the COM-Poisson with varying dispersion is a fully parametric model that has the advantages of allowing predictions for probabilities and further generalizations such as the inclusion of random effects and modelling of censored data.

4 Estimation and inference

To fit COM-Poisson models with varying dispersion, we use the maximum likelihood and inferences are based on the standard asymptotic likelihood theory. The log-likelihood function for $\boldsymbol{\theta} = (\boldsymbol{\beta}^\top, \boldsymbol{\gamma}^\top)^\top$ parameters is given by

$$\ell = \ell(\boldsymbol{\theta}; \boldsymbol{y}) = \sum_{i=1}^{n} \left\{ \nu_i \log\left(\mu_i + \frac{\nu_i - 1}{2\nu_i}\right) - \nu_i \log(y_i) - \log[Z(\mu_i, \nu_i)] \right\}, \tag{2}$$

where $\mu_i = \exp(\boldsymbol{x}_i^\top \boldsymbol{\beta})$, $\nu_i = \exp(\boldsymbol{z}_i^\top \boldsymbol{\gamma})$, and $Z(\mu_i, \nu_i)$ is the normalizing constant computed for the parameters μ_i and ν_i.

Parameter estimation requires the numerical maximization of Equation (2). Since the derivatives of ℓ cannot be obtained in closed forms, we compute them by central

finite differences using the Richardson method as implemented in the package `numDeriv` (Gilbert & Varadhan 2016) for the statistical software `R` (R Core Team 2018).

Standard errors for the parameter estimates are obtained based on the observed information matrix. Using derivatives of ℓ computed at the maximum likelihood estimates, the variance-covariance matrix of the maximum likelihood estimators may be expressed as

$$\boldsymbol{V}_\theta = \begin{pmatrix} -\partial\ell^2/\partial\boldsymbol{\beta}\partial\boldsymbol{\beta}^\top & -\partial\ell^2/\partial\boldsymbol{\beta}\partial\boldsymbol{\gamma}^\top \\ -\partial\ell^2/\partial\boldsymbol{\gamma}\partial\boldsymbol{\beta}^\top & -\partial\ell^2/\partial\boldsymbol{\gamma}\partial\boldsymbol{\gamma}^\top \end{pmatrix}^{-1} = \begin{pmatrix} \boldsymbol{V}_\beta & \boldsymbol{V}_{\beta\gamma} \\ \boldsymbol{V}_{\gamma\beta} & \boldsymbol{V}_\gamma \end{pmatrix}.$$

Based on the asymptotic distribution of the maximum likelihood estimators, we can obtain the variances for $\hat{\eta}_i$ and $\hat{\xi}_i$ using the delta method, $\text{Var}(\hat{\eta}_i) = \boldsymbol{x}_i^\top \boldsymbol{V}_{\beta|\gamma}\boldsymbol{x}_i$ and $\text{Var}(\hat{\xi}_i) = \boldsymbol{z}_i^\top \boldsymbol{V}_{\gamma|\beta}\boldsymbol{z}_i$, where $\boldsymbol{V}_{\beta|\gamma} = \boldsymbol{V}_\beta - \boldsymbol{V}_{\beta\gamma}\boldsymbol{V}_\gamma^{-1}\boldsymbol{V}_{\gamma\beta}$ and $\boldsymbol{V}_{\gamma|\beta} = \boldsymbol{V}_\gamma - \boldsymbol{V}_{\gamma\beta}\boldsymbol{V}_\beta^{-1}\boldsymbol{V}_{\beta\gamma}$. Since $\boldsymbol{\beta}$ and $\boldsymbol{\gamma}$ were found to be nearly orthogonal, $\boldsymbol{V}_{\beta\gamma} = \boldsymbol{V}_{\gamma\beta}^\top \approx \boldsymbol{0}$, hence $\boldsymbol{V}_{\beta|\gamma} \approx \boldsymbol{V}_\beta$ and $\boldsymbol{V}_{\gamma|\beta} \approx \boldsymbol{V}_\gamma$, which implies that inferences based on the conditional log-likelihood and the marginal log-likelihood are the same.

Confidence intervals for μ_i and ν_i are obtained by back-transforming the confidence intervals for η_i and ξ_i. Maximum likelihood estimation for fitting COM-Poisson models and methods for computing the associated confidence intervals are implemented in the `cmpreg`[1] `R` package.

5 Data analysis

5.1 Analysis of nitrofen experiment

To analyse the number of live offspring under different doses of nitrofen for the mean we use a cubic polynomial in `dose` and a similar model for the dispersion

$$\log(\nu_{ij}) = \gamma_0 + \gamma_1 \mathtt{x}_{1i} + \gamma_2 \mathtt{x}_{2i}^2 + \gamma_3 \mathtt{x}_{3i}^3, i = 1, 2, 3, 4, 5 \quad \text{and} \quad j = 1, 2, \ldots, 10$$

where i and j refer to the nitrofen concentration level (`dose`) and to the replicates, respectively. For the dispersion we also consider nested submodels: i.e. constant, linear, and quadratic.

Table 1 shows the goodness-of-fit measures and comparison of nested models for the dispersion. There is clear evidence that the linear predictor for the dispersion is at least linearly dependent on the nitrofen concentration level. However, there is no clear evidence to decide between linear and quadratic models for the dispersion.

Table 1: Nitrofen data: goodness-of-fit measures (deviance and AIC) and model comparisons (based on deviance differences, Δ-Dev) of the dispersion models.

	df	Deviance	AIC	Δ-Dev	$\Pr(>\chi^2)$
Constant	45	288.127	298.127		
Linear	44	274.111	286.111	14.0164	0.0002
Quadratic	43	270.493	284.493	3.6179	0.0572
Cubic	42	269.503	285.503	0.9898	0.3198

Deviance is computed as minus twice log-likelihood

[1] Available on GitHub `https://github.com/jreduardo/cmpreg`

Table 2: Nitrofen data: Parameter estimates (Est) and standard errors (SEs) for the fitted double regression COM-Poisson model.

	Estimates (Standard Errors)			
Parameter	Constant	Linear	Quadratic	Cubic
Mean				
β_0	3.4769 (0.0541)[a]	3.4778 (0.0283)[a]	3.4777 (0.0339)[a]	3.4776 (0.0360)[a]
β_1	−0.0879 (0.1943)	−0.1055 (0.1424)	−0.1167 (0.1322)	−0.1153 (0.1283)
β_2	0.1547 (0.1731)	0.1747 (0.1492)	0.1917 (0.1375)	0.1886 (0.1318)
β_3	−0.0976 (0.0396)[a]	−0.1028 (0.0380)[a]	−0.1082 (0.0368)[a]	−0.1069 (0.0350)[a]
Dispersion				
γ_0	0.0474 (0.2047)	0.2948 (0.2112)	0.2437 (0.2589)	0.3532 (0.2268)
γ_1	–	−5.2441 (1.3630)[a]	−7.0024 (2.3054)[a]	−5.7301 (1.8440)[a]
γ_2	–	–	−3.9807 (2.4439)	−2.9175 (1.9045)
γ_3	–	–	–	1.5221 (1.4119)

Est (SE)[a] indicates |Est/SE| > 1.96.

The estimated parameters, their associated standard errors and individual Wald tests are presented in Table 2. Note that the parameters estimated in the mean structure are very close across the different models considered for the dispersion. This arises due to the orthogonality property of the μ_i and ν_i parameters. For the dispersion structure, there is no evidence to keep the quadratic term, the Wald statistics is -1.63 (p-value $= 0.1034$), but note that the mean model parameter standard errors do change (decrease) once the linear term is included in the dispersion.

Figure 3(a, b) present the fitted values with confidence bands for the mean model and linear and quadratic dispersion models. When we use a constant dispersion, the fitted model suggests equidispersion ($\nu = 1$), with $\exp(\hat{\gamma}_0) = \exp(0.0474) = 1.049$. However, when we relax this assumption, it is clear that the dispersion changes across nitrofen levels. In particular, all models show that at around $2\mu g/10^2$ litre, the number of live offspring change from under- to over-dispersed.

The variances for nitrofen doses obtained from the fitted models with linear and quadratic models for the dispersion are presented in Figure 3(c). The model with a linear predictor for the dispersion does not fit the sample variances for the doses 1.6 and $2.35\mu g/10^2$ litre well. The model with a quadratic predictor fits these variances better, however, it produces rather strange behaviour for values greater than $2.35\mu g/10^2$ litre, suggesting over-fitting.

5.2 Analysis of the soybean experiment

In the analysis of the number of pods under different potassium fertilizer (K) and soil moisture levels, we consider the follow mean and dispersion linear predictors:

$$\log(\mu_{ijk}) = \beta_0 + \kappa_i + \tau_j + (\beta_1 + \delta_j)\mathtt{K}_k + \beta_2^2\mathtt{K}_k^2,$$
$$\log(\nu_{ijk}) = \alpha_j + \gamma_1\mathtt{K}_k,$$

where i, j, and k are indices for block, moisture level, and potassium dose. Note that for the dispersion, the α_j is the logarithm of dispersion parameter when the potassium dose is 0 (without an intercept term).

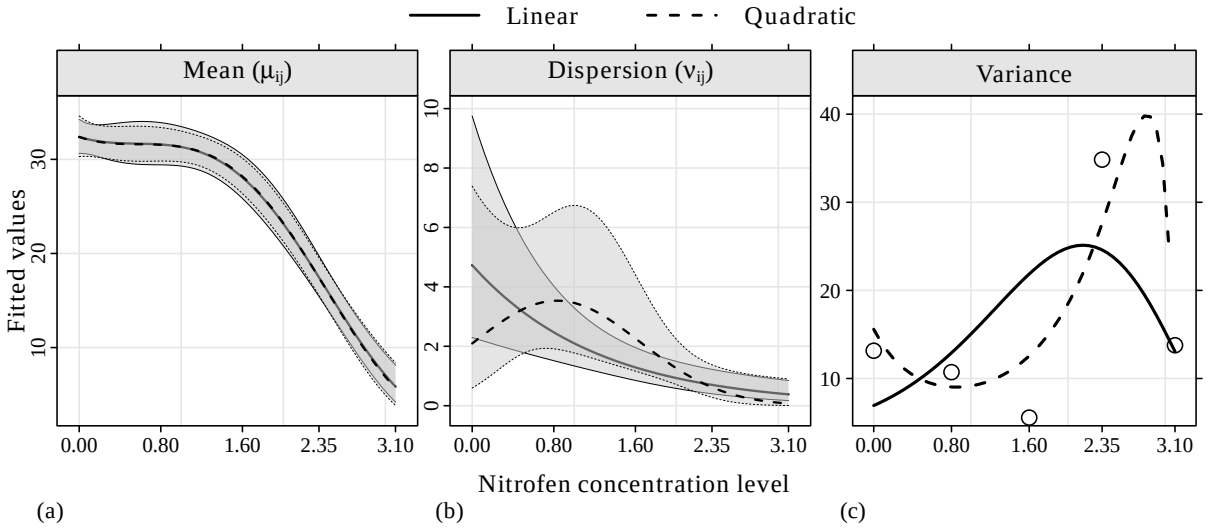

Figure 3: (a-b) Fitted values for mean and dispersion parameters with 95% confidence bands and (c) variances obtained from the fitted models. The line types indicate the linear predictor considered.

Table 3: Soybean data: goodness-of-fit measures (deviance and AIC) and model comparisons (based on deviance differences, Δ-Dev) of the dispersion models.

	df	Deviance	AIC	Δ-Dev	$\Pr(>\chi^2)$
Constant	62	534.232	558.232		
Moisture	60	527.866	555.866	6.3658	0.0415
Moisture + K	59	525.848	555.848	2.0181	0.1554

Deviance is computed as minus twice log-likelihood

Table 3 shows the goodness-of-fit measures and comparison of the full additive dispersion model (moisture + K) with the reduced models (i) $\gamma_1 = 0$ (moisture effect) and (ii) $\alpha_j = \alpha$ and $\gamma_1 = 0$ (constant). The results show a significant improvement in varying the dispersion for each moisture level but do not present any clear evidence for the relation between the dispersion and the potassium doses when moisture is already included in the model.

Table 4 gives the parameter estimates and associated standard errors for the three different models. It seems that the mean structure is well specified since the Wald tests lead to the same conclusions across the different dispersion structures. The likelihood ratio tests indicate that we have different dispersion levels for each moisture level. In particular, considering the reduced model $\gamma_1 = 0$, the fitted dispersions values for each moisture level are $\hat{\nu}_{37.5\%} = 0.701$, $\hat{\nu}_{50.0\%} = 0.742$, and $\hat{\nu}_{63.5\%} = 1.99$. The point estimates indicate overdispersion for the two first and underdispersion for the latter.

The individual 95% confidence intervals for the dispersion components are shown in Figure 4. The intervals are obtained by working with the profile deviance function with respect to each α_j. The results indicate neither under- nor overdispersion for moisture levels 37.5% and 50%. For the level 63.5%, there is marginal evidence for underdispersion, although the lower bound is close to zero, however there is evidence that this group differs from the other two.

The observed and fitted counts for each moisture level with associated confidence

Table 4: Soybean data: Parameter estimates (Est) and standard errors (SEs) for the fitted double regression COM-Poisson model.

	Estimates (Standard Errors)		
Parameter	Constant	Moisture	Moisture + K
Mean			
β_0	4.0062 (0.0544)[a]	4.0112 (0.0576)[a]	4.0273 (0.0632)[a]
κ_{II}	−0.0293 (0.0426)	−0.0320 (0.0381)	−0.0398 (0.0359)
κ_{III}	−0.0727 (0.0431)	−0.0991 (0.0393)[a]	−0.1097 (0.0379)[a]
κ_{IV}	−0.1254 (0.0437)[a]	−0.1452 (0.0403)[a]	−0.1573 (0.0380)[a]
κ_{V}	−0.1037 (0.0446)[a]	−0.0960 (0.0411)[a]	−0.1016 (0.0394)[a]
$\tau_{50.0\%}$	0.1573 (0.0583)[a]	0.1571 (0.0659)[a]	0.1557 (0.0723)[a]
$\tau_{63.5\%}$	0.1730 (0.0582)[a]	0.1731 (0.0562)[a]	0.1758 (0.0610)[a]
β_1	0.5851 (0.0902)[a]	0.5976 (0.0858)[a]	0.5596 (0.0898)[a]
$\delta_{50.0\%}$	0.1469 (0.0552)[a]	0.1471 (0.0625)[a]	0.1484 (0.0600)[a]
$\delta_{63.5\%}$	0.1398 (0.0553)[a]	0.1407 (0.0539)[a]	0.1374 (0.0511)[a]
β_2	−0.2683 (0.0434)[a]	−0.2751 (0.0387)[a]	−0.2545 (0.0397)[a]
Dispersion			
$\alpha_{37.5\%}$	−0.0826 (0.1652)	−0.3546 (0.3145)	−0.7023 (0.4067)
$\alpha_{50.0\%}$	–	−0.2979 (0.2982)	−0.6413 (0.3979)
$\alpha_{63.5\%}$	–	0.6893 (0.3023)[a]	0.4615 (0.3459)
γ_1	–	–	0.4314 (0.2983)

Est (SE)[a] indicates |Est/SE| > 1.96.

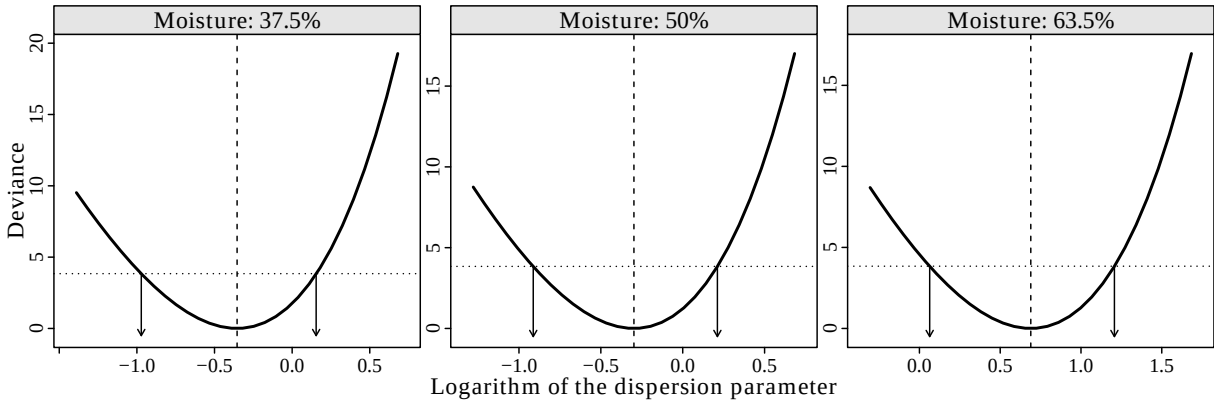

Figure 4: Profile deviance for each dispersion component and their respective 95% confidence intervals.

intervals are shown in Figure 5, along with the optimum doses. The results show that potassium doses at 104.21, 132.63 and 132.63mg dm^{-3} lead to the expected maximum number of pods for the moisture levels 37.5%, 50%, and 62.5%, respectively. In terms of the number of pods, there is evidence that fertilizing with potassium can compensate for a water deficit in soybean culture.

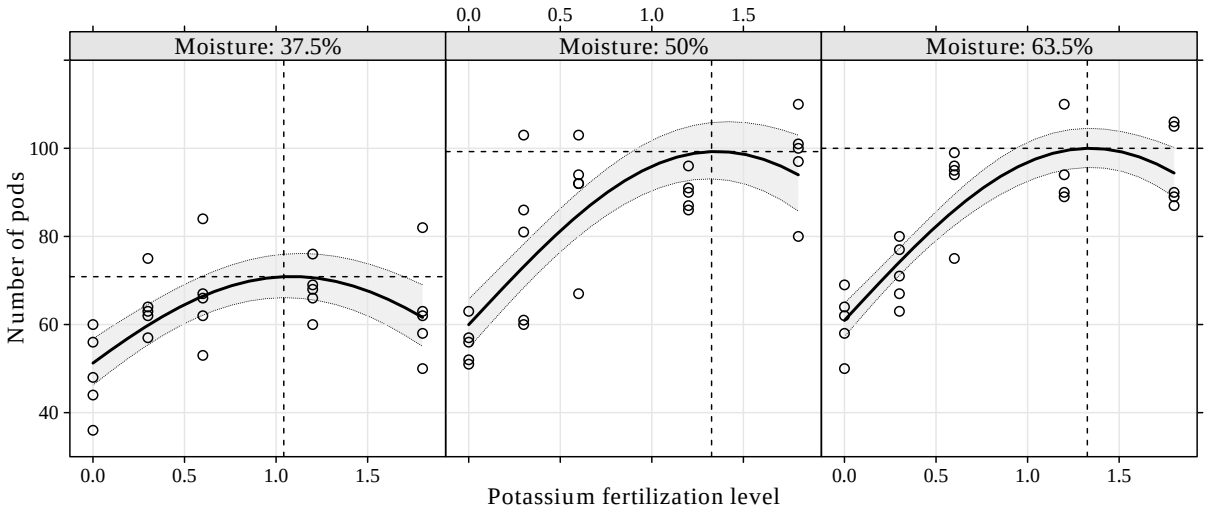

Figure 5: Fitted values for mean and dispersion parameters with 95% confidence bands. Dotted lines indicate the optimal doses and the corresponding expected number of pods

6 Discussion

In this paper, COM-Poisson models with varying dispersion were proposed for jointly modelling mean and dispersion in the analysis of counts with different levels of dispersion. This class of models allows the dispersion to depend on covariates. The parameters are estimated by maximum likelihood and inferences are made based on the usual asymptotic theory..

The methodology is applied to analyse two count datasets obtained from planned experiments. The proposal presented improvements in terms of data fitting when compared to the conventional COM-Poisson with constant dispersion. In particular, under this methodology, we are able to analyse the effects of experimental (observational) conditions in the dispersion as well as in the mean.

For future work, simulation studies are required to evaluate the robustness of the model. In addition, as an improvement for the case study analyses, considering nonlinear, or smooth, predictors for the mean could be useful in order to avoid the use of higher-order polynomials, as well as imposing biological constraints on the model.

Acknowledgements

This work was partially supported by CNPq and by FAPESP, Brazilian science funding agencies.

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