Estimation of the Discrete Log-normal Model

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1 Introduction

Count data arise frequently in many scientific and industrial settings. Often, the Poisson model serves as the starting point for analyzing these data sets, due largely to its simplicity and interpretability. However, it assumption of equidispersion often proves problematic.

In many applications, data analysts find that the variance of their collected data set is substantially larger than the mean, a situation referred to as overdispersion. Historically, overdispersion has received a great deal of attention due to (1) its ubiquity and (2) theoretical reasons why it might occur (see, for example, the discussion in [5]). Underdispersion, though less common, can also have undesirable implications for statistical analysis (see [7] for models designed to address this problem).

Relatively few count models work well for both underdispersion and overdispersion, and each has its own drawbacks. For example, the quasipoisson model does not involve a true likelihood function, which may be undesirable for certain use cases; e.g., generating prediction intervals. As another example, the COM-Poisson model is extremely flexible and a member of the exponential family; however, its moments are not available in closed form and must be approximated.

In this project, we explore a flexible and straightforward model count model that Easton proposed in STATS 608 and fit using Bayesian methods. We call it the discrete log-normal (DLN) model because it involves a latent log-normal random variable that is discretized in a deterministic fashion. In Section 2, we motivate and formulate the model. In Section 3, we propose two families of methods for fitting the model. In Section 4, we apply the methods to simulated data sets. We close with a discussion of the results in Section 5.

2 Statistical Model

Mathematically, the DLN model takes the following form:

$$Y_i = \lfloor \exp(Z_i) \rfloor, \quad Z_i \sim \text{Normal}(\mu_i, \sigma_i), \quad \mu_i = x_i'\beta, \quad \sigma_i = \exp(w_i'\alpha) \tag{1}$$

The model uses a vector generalized linear model [6] (VGLM) for a latent variable, Z_i. The variable Z_i is then exponentiated and rounded down to obtain a count, $Y_i \in \{0, 1, 2, ...\}$. x_i is a vector of predictors for the mean function and w_i is a vector of predictors for the variance function. While unconventional, the model offers at least four compelling benefits:

1. The model naturally allows for underdispersion and overdispersion by adjusting the magnitude of α
2. The model is not restricted to a fixed mean-variance relationship; instead it allows the variance to change as a flexible function of predictor variables
3. Algorithms for fitting this model are straightforward because of the latent Gaussian structure
4. The latent Gaussian structure also facilitates various extensions (e.g., dependent data structures or zero-inflation via a mixture model)

3 Optimization Algorithms

We fit the model in Section 2 using L_2-penalized maximum likelihood estimation. We use two broad families of optimization algorithms to fit the model. The first family directly optimizes the loss function using gradient-based methods. The second uses the the expectation-maximization algorithm (see [2] for an overview of this algorithm). We discuss these families of algorithms in detail in Sections 3.1 and 3.2, respectively.

3.1 Direct Gradient-Based Methods

The gradient derivations for the first two model-fitting approaches are facilitated by writing the marginal likelihood of Y_i as follows:

$$p\left(y_i \mid \alpha, \beta\right) = \int_{\log(y_i)}^{\log(y_i+1)} f(t \mid \mu_i, \sigma_i)\, dt = F\left\{\log(y_i+1) \mid \mu_i, \sigma_i\right\} - F\left\{\log(y_i) \mid \mu_i, \sigma_i\right\} \tag{2}$$

Where f and F denote the pdf and cdf of the normal distribution with parameters μ_i and σ_i. The penalized log-likelihood function is then given by

$$\ell(\alpha, \beta) = \sum_{i=1}^{n} \log p\left(y_i \mid \alpha, \beta\right) - \frac{\lambda}{2}\left(\alpha'\alpha + \beta'\beta\right) \tag{3}$$

For simplicity, we employ a single penalization parameter, λ, in our derivations. However, data analysts can enforce differing levels of penalization by either (a) rescaling their covariates or (b) making straightforward adjustments to the provided formulas. As is typical, we omit the penalty for the intercept in β; however, we include it for the intercept in α because doing so improves the stability of our model-fitting algorithms. The gradient and Hessian of $\ell(\alpha, \beta)$ are provided in Appendix B. With these computations in hand, we can easily use a variety of gradient-based optimization routines.

We implemented these methods by extending the GenericLikelihoodModel class in the `statsmodels` package in Python [3]. The GenericLikelihoodModel class allows the fitting of any likelihood function via maximum likelihood estimation. After implementing class methods for the (potentially penalized) likelihood function, gradient, and Hessian, this class allows the user to optimize their likelihood function using many pre-configured routines, including the Nelder-Mead, Powell, BFGS, conjugate gradient, Newton-conjugate gradient, and classic Newton methods.

The greatest challenge in using these direct gradient-based approaches is that the gradients and Hessians involve dividing very small terms, which can easily result in catastrophic cancellation. Appendix B explains how to mitigate this challenge by performing calculations on the log scale. We also found that using starting values from a standard Poisson GLM (for β) made our algorithms more likely to converge without errors.

3.2 Expectation Maximization Algorithms

Expectation maximization algorithms for our model involve calculating the expected penalized log-likelihood of Y and Z, fixing the parameters to their current working estimates. The expectation is taken with respect to the distribution of the Z given both the parameters and Y. Because the full expectation decomposes as a sum of expectations of i, it suffices to compute the distribution for one value of i. This conditional turns out to be a truncated normal distribution. The details of this result and other technical results in this section are available in Appendix C.

The expectation of interest involves the moments of a truncated normal distribution which, conveniently, are available in closed form. Denoting the first and second moments of this distribution as e_{1i} and e_{2i}, the full expectation becomes

$$h(\alpha, \beta) = \sum_{i=1}^{n} \Big[-\log(\sigma_i) - \frac{1}{2\sigma_i^2}\big(e_{2i} - 2\, e_{1i}\, \mu_i + \mu_i^2\big)\Big] - \frac{\lambda}{2}\left(\beta'\beta + \alpha'\alpha\right) \tag{4}$$

The next step of the algorithm is to maximize this quantity with respect to α and β. Comparing this equation to the log-likelihood function for normal linear regression, we see that the optimal value of β is given by an L^2-penalized weighted least squares regression, the solution to which is given by

$$\hat{\beta} = \left(X'\Sigma^{-1}X + \lambda I\right)^{-1} X'\Sigma^{-1}e_1 \tag{5}$$

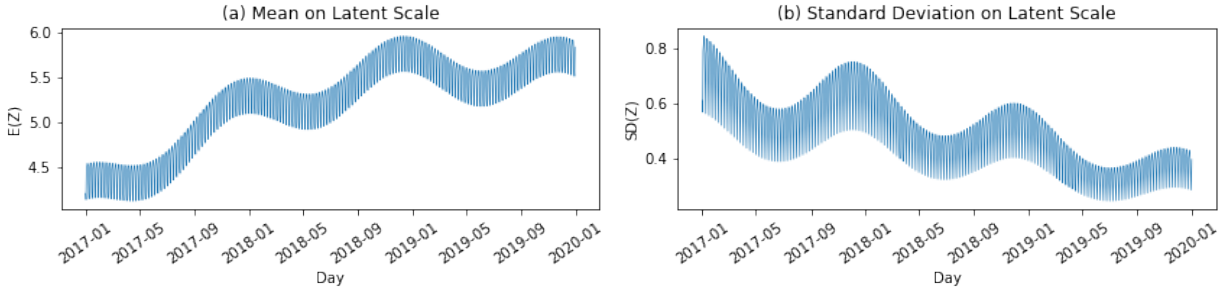
Where Σ is a diagonal matrix with the i-th diagonal element equal to σ_i^2 and e_1 is a column vector with i-th element e_{1i}. In contrast, the optimal value of α does not have a simple closed-form solution. Instead, we must use gradient-based optimization techniques such as those applied in 3.1. We tested two optimization algorithms for this problem: a first-order version using gradient ascent with back-tracking line search and a second-order version using Newton's method.

4 Results

In this section, we simulate data from our model and estimate its parameters using the techniques discussed in Section 3. The model structure for our simulation is based on time series count data, which arise commonly in online web-tracking. A typical objective in this setting is to generate short-horizon (e.g., one-week) predictions and prediction intervals in order to identify 'anomalies' in incoming data.

In our simulations, the predictors for the mean function are the same as the predictors for the variance function; i.e., $x_i = w_i$. Each covariate vector is composed of an intercept, quadratic time trend, day-of-the-week indicators, and two trigonometric functions to induce seasonality—giving 22 parameters in total. Their values were selected such that (1) the resulting time series are similar to those observed in practice and (2) the mean-variance relationship is more sophisticated than typical count models allow. Note in Figure 1 that, although the mean of the latent variable Z generally increases over time, its standard deviation decreases.

Figure 1: The mean (a) and standard deviation (b) of our latent variable Z under the true parameters in our simulations.



Sections 4.1 and 4.2 examine the performance of our model and algorithms on 100 simulated time series data sets. Section 4.1 compares the performance of the true model to some competing models, and Section 4.2

compares our proposed algorithms in terms of their empirical convergence and runtime. In both sections, we impose a small penalty of only 10^{-4}.

4.1 Model Comparison Case Study

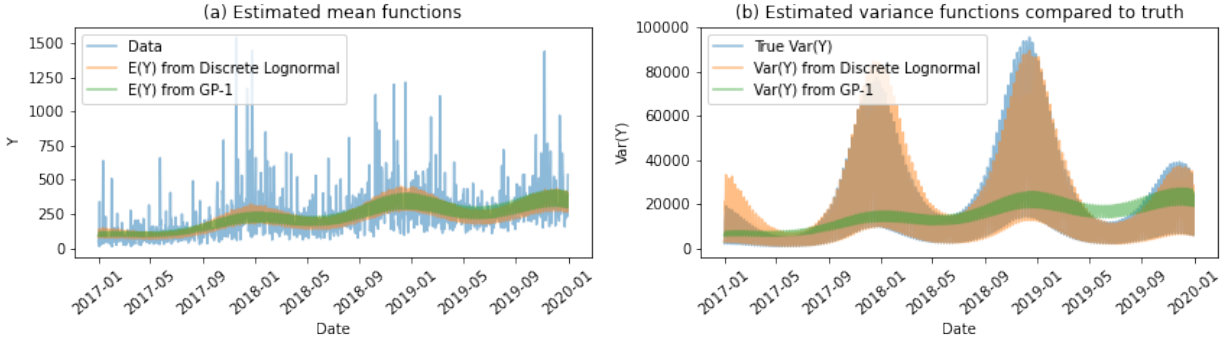
Here we compare our discrete log-normal model (DLN) to three other models commonly used to model count data: The standard Poisson GLM (POI), the generalized Poisson 1 (GP-1) model, and the negative binomial 1 (NB-1) models. We fit each model to 100 simulated time series data sets and test the models' mean squared prediction error (MSPE) on a new data set. The results from our simulation are summarized in Table 1.

Discrete Model	DLN	POI	GP-1	NB-1
MSPE	**20,629**	20,677	21,258	20,892
Standard Deviation	3,022	3,030	3,158	3,116

Table 1: Table showing the mean squared prediction error for four different models fit to the data: discrete log-normal (DLN), poisson (POI), generalized poisson (GP-1), and negative binomial (NB-1).

As expected, the DLN performs best because it is the only model capable of capturing the true variance function. Figure 2 shows the estimated means and variances of the DLN model compared to the GP-1 model. Plot (a) shows that estimated mean functions closely track each other and the data, and plot (b) shows that the GP-1 model is not capable of capturing the true variance function because it assumes that the mean and variance are proportional.

Figure 2: Plot (a) shows the estimated mean functions from the DLN and GP-1 models fit to the data set shown in blue. Plot (b) shows the estimated variance functions fit to the same data, along with the true variance function shown in blue.

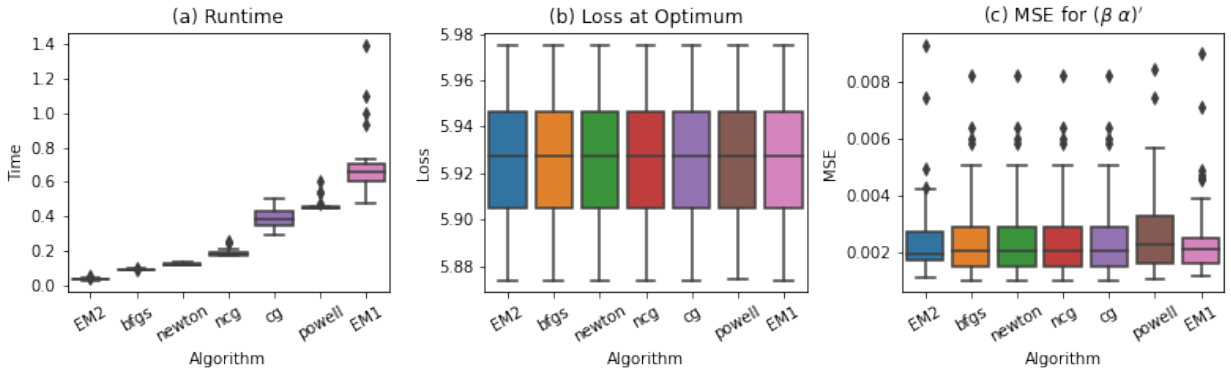


4.2 Algorithm Comparison Simulation

In this section, we again generate 100 time series data sets from our model. We then fit the discrete log-normal model using the seven optimization algorithms given in Section 3. We ran each algorithm until the penalized log-likelihood (given in Equation (3)) improved by less than 10^{-8}.

The results are summarized in Figure 3 and Table 2. Plot (a) in Figure 3 visually compares the runtimes for the different algorithms, and the table shows the mean runtime for each algorithm. These results show that the fastest algorithm is the second-order EM algorithm, which takes less than half as much time as the

Figure 3: Comparison of the algorithms given in Section 3 on 100 simulated data sets. Plot (a) shows a great deal of variation in runtime among the algorithms with the second-order EM algorithm (EM2) performing the best. On the other hand, plots (b) and (c) provide evidence that the algorithms converge to nearly identical solutions because they achieve similar losses (a) and MSE in estimating the parameters (b).



Algorithm	EM2	bfgs	newton	ncg	cg	powell	EM1
Mean Runtime (sec)	0.042	0.098	0.126	0.192	0.392	0.464	0.703

Table 2: Table showing the mean runtimes for the seven algorithms compared in our simulation study, sorted by the mean runtime.

next two fastest algorithms: BFGS and the Newton method. The first-order EM algorithm is the slowest algorithm, probably because the back-tracking line search is a time-consuming process.

Plots (b) and (c) in the figure compare the algorithms in terms of the quality of their returned solutions. Plot (b) shows the negative penalized log-likelihood (labeled as "Loss" for brevity). The fact that these boxplots are almost visually indistinguishable provides evidence that all seven algorithms are converging to equally good solutions. Plot (c) shows the MSE in estimating α and β. We see more variability in this plot than in plot (b); however, the differences are likely negligible, especially in view of the similar loss values.

5 Discussion

In this project, we explored a new and extremely flexible statistical model for count data, and we derived two general families of methods for fitting the model via penalized maximum likelihood estimation: (1) direct gradient-based methods and (2) EM algorithms. In our simulations, we found that both approaches perform well but that the second-order EM algorithm is the most computationally efficient (at least for the size of data we were using). Second-order methods often scale poorly with data size, especially in high dimensions, so the first-order methods may be preferable with larger data sets.

One exciting avenue for future research would be to extend the discrete log-normal model to allow for correlation between the observations. This change could be accommodated by introducing correlation into the latent Gaussian variable Z. Adapting the EM algorithm to account for this change would be particularly straightforward. The E-step would require calculating expectations with respect to a truncated multivariate Gaussian distribution (for which there are readily available algorithms and software [4]). The update for β would remain essentially unchanged (though Σ would no longer be diagonal). The gradient and Hessian for α would require a bit more effort, but should also be tractable.

References

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A Contributions

Easton's contributions:

- Wrote project proposal
- Derived gradients, Hessian, and EM algorithms
- Wrote code for implementing EM algorithms
- Took the lead on structuring the paper

Mason's contributions:

- Wrote code for fitting the proposed model via direct gradient-based methods
- Wrote sections in the paper about direct gradient-based methods and model comparisons
- Took the lead on peer review

B Gradient and Hessian Calculations

We drop the i subscript in this section for simplicity. We also define the following quantities for ease of notation:

- $\underline{z} = (\log(y) - \mu)/\sigma$
- $\bar{z} = (\log(y+1) - \mu)/\sigma$
- $\Phi(\cdot)$: Standard normal cdf
- $\phi(\cdot)$: Standard normal pdf
- $\kappa_q = \dfrac{\bar{z}^q\,\phi(\bar{z}) - \underline{z}^q\,\phi(\underline{z})}{\Phi(\bar{z}) - \Phi(\underline{z})}$, for $q \in \{0, 1, 2, 3\}$

Working from equation (2), the gradient of $\log p\,(y_i \,|\, \alpha, \beta)$ with respect to β is

$$\nabla_\beta \log p\,(y \,|\, \alpha, \beta) = -\frac{\kappa_0}{\sigma} x \tag{6}$$

Similarly, the gradient with respect to α is

$$\nabla_\alpha \log p\,(y \,|\, \alpha, \beta) = -\kappa_1 w \tag{7}$$

Using these derivations, it's straight forward to calculate the gradient with respect to the penalized log-likelihood $\ell(\alpha, \beta)$ is:

$$\begin{aligned} \nabla_\beta\, \ell(\alpha, \beta) &= -\sum_{i=1}^{n} \frac{\kappa_{0i}}{\sigma_i} x_i - \lambda\,\beta \\ \nabla_\alpha\, \ell(\alpha, \beta) &= -\sum_{i=1}^{n} \kappa_{1i} w_i - \lambda\,\alpha \end{aligned} \tag{8}$$

Similar calculations yield the Hessian:

$$\frac{\partial}{\partial\beta\partial\beta'}\, \ell(\alpha, \beta) = -\sum_{i=1}^{n} \frac{\kappa_{0i}^2 + \kappa_{1i}}{\sigma_i^2} x_i x_i' - \lambda\, I \tag{9}$$

$$\frac{\partial}{\partial\beta\partial\alpha'}\, \ell(\alpha, \beta) = -\sum_{i=1}^{n} \frac{\kappa_{2i} + \kappa_{0i}\,(\kappa_{1i} - 1)}{\sigma_i}\, x_i w_i' \tag{10}$$

$$\frac{\partial}{\partial\alpha\partial\alpha'}\, \ell(\alpha, \beta) = -\sum_{i=1}^{n} [\kappa_{1i}\,(\kappa_{1i} - 1) + \kappa_{3i}]\, w_i w_i' - \lambda\, I \tag{11}$$

One potential challenge in performing these calculations is that the numerator and denominator in κ_q are often quite small, so a naive implementation can easily result in divide-by-zero errors as the denominator

could, without too much difficulty, be computationally zero. One way of circumventing this issue is to perform the calculations on the log scale. Doing so requires carefully using the following identity for both numerator and denominator: Given $0 < a < b$,

$$\log(b - a) = \log\left[a(b/a - 1)\right] = \log(a) - \log(b/a - 1) \tag{12}$$

The ratio b/a can also be written as $\exp\{\log(b) - \log(a)\}$. Taken together, these identities allow one to compute κ_q using the log-PDF and log-CDF of the normal distribution, both of which are readily available in common statistical computing environments. These tricks do not avoid all computational challenges associated with calculating κ_q, but we found that they noticeably reduce the potential for errors.

C Expectation-Maximization Details

In this section, we present the details of our L_2-regularized EM algorithm. The E-step in our algorithm involves calculating the following expectation:

$$h(\alpha, \beta) = \sum_{i=1}^{n} \mathbb{E}_{Z_i \sim q} \log p(Z_i, y_i | \theta) - \frac{\lambda}{2}\big(\alpha'\alpha + \beta'\beta\big) \tag{13}$$

Where $q = p(Z_i | \alpha, \beta, Y_i)$. We can work out this distribution as follows:

$$\begin{aligned} & p(z_i \,|\, \alpha, \beta, y_i) \\ \propto\; & p(z_i \,|\, \alpha, \beta)\, p(y_i \,|\, z_i) \\ =\; & \text{Normal}(\mu_i, \sigma_i^2)\, \text{I}\{y_i = \lfloor \exp(z_i) \rfloor\} \end{aligned} \tag{14}$$

Thus, given $Y_i = y_i$, Z_i follows a truncated normal distribution with parameters μ_i, σ_i^2, $\log(y_i)$, and $\log(y_i{+}1)$, where the latter two parameters indicate the interval of truncation. Calculating the above expectation requires the first and second moments of a truncated normal random variable which can be found in section 10.1 of [1]. They involve the ratios κ_0 and κ_1 defined in the previous appendix. For brevity, we denote these first and second moments (which depend on parameter estimates from the previous iteration of the EM algorithm) as e_{1i} and e_{2i}, respectively. Equation (4) then follows from this result. The optimal value for β given in Equation (5) can then be found by taking derivatives and setting them to zero.

We now provide the gradient and Hessian of $h(\alpha, \beta)$ with respect to α:

$$\begin{aligned} \nabla_\alpha h(\alpha, \beta) &= W'(\Sigma^{-1}c - \mathbb{1}) - \alpha \\ \frac{\partial}{\partial \alpha \partial \alpha'}\, h(\alpha, \beta) &= -2W'\Sigma^{-1}CW - \lambda I \end{aligned} \tag{15}$$

Where C is a diagonal matrix with i-th element equal to $e_{2i} - 2\, e_{1i}\, \mu_i + \mu_i^2$, $c = \text{diag}(C)$, and $\mathbb{1}$ is a vector of ones. As mentioned in the main text, we use these results to run two versions of the EM algorithm: a first-order version using gradient ascent with back-tracking line search and a second-order version using Newton's method. With each method, we update α only once per iteration of the EM algorithm.

In our gradient ascent algorithm, we employed a step-size of 0.001. In the back-tracking line search, we cut the step size in half until achieving our sufficient ascent condition, which required that $h(\alpha, \beta)$ improve by at least half of the amount predicted by a first order Taylor series; i.e., until

$$h\left(\hat{\alpha}^{(t)} + \eta\, d^{(t)},\ \hat{\beta}^{(t)}\right) - h\left(\hat{\alpha}^{(t)},\ \hat{\beta}^{(t)}\right) \geq \frac{\eta}{2} ||d^{(t)}||_2^2 \tag{16}$$

Where $\hat{\alpha}^{(t)}$ and $\hat{\beta}^{(t)}$ denote the estimates of α and β at iteration t in the EM algorithm, η is the step size, and $d = \nabla_\alpha h(\alpha, \beta)|_{\alpha = \hat{\alpha}^{(t)}, \beta = \hat{\beta}^{(t)}}$.

The Newton algorithm was much more straightforward. In each iteration of the EM algorithm, we set $\hat{\alpha}^{(t+1)}$ as follows:

$$\hat{\alpha}^{(t+1)} = \hat{\alpha}^{(t)} + \left(Q^{(t)}\right)^{-1} d^{(t)} \tag{17}$$

Where $Q^{(t)} = \frac{\partial}{\partial \alpha \partial \alpha'} h(\alpha, \beta)|_{\alpha=\hat{\alpha}^{(t)}, \beta=\hat{\beta}^{(t)}}$, the form of which is given in equation (15).

With both of these methods, we opted to update α only once per iteration of the EM algorithm. Doing so resulted in satisfactory convergence and, at least for the second-order method, competitive runtimes compared to the direct gradient-based methods.