Notes on Hurdle Negative Binomial Regression

ADAM KAPELNER¹

¹Department of Mathematics, Queens College, CUNY, USA

August 20, 2023

We begin with examining the zero-inflated model and then talk about why it's wiser to go with the hurdle model.

So we start by modeling count data using a negative binomial model where the zeroes are inflated. Let inflation be defined as the latent variable $I_i = 1$ and uninflated be $I_i = 0$. We first define the probability p_i of an inflated zero using a generalized linear model (GLM) as

$$p_i := \mathbb{P}(Y_i = 0 \mid I_i = 1) := (1 + \exp(-\eta_i))^{-1}$$

where

$$\eta_i := \gamma_0 + \gamma_1 x_{i,1} + \ldots + \gamma_p x_{i,p}$$

and conveniently

$$1 - p_i = (1 + \exp(\eta_i))^{-1}.$$

We then define the count model for y_i which is uninflated $I_i = 0$ as the negative binomial model parameterized with the mean as stated here and a generalized linear model (GLM):

$$\mathbb{P}(Y_i = y_i \mid I_i = 0) = \begin{pmatrix} y_i + \phi - 1 \\ y_i \end{pmatrix} \left(\frac{\mu_i}{\mu_i + \phi}\right)^{y_i} \left(\frac{\phi}{\mu_i + \phi}\right)^{\phi} \\
= \frac{\Gamma(y_i + \phi - 2)}{y_i! \Gamma(\phi - 2)} \left(\frac{\mu_i}{\mu_i + \phi}\right)^{y_i} \left(\frac{\phi}{\mu_i + \phi}\right)^{\phi} \\
= \frac{\Gamma(y_i + \phi - 2)}{y_i! \Gamma(\phi - 2)} \left(\frac{\exp(\xi_i)}{\exp(\xi_i) + \phi}\right)^{y_i} \left(\frac{\phi}{\exp(\xi_i) + \phi}\right)^{\phi} \\
= \frac{\Gamma(y_i + \phi - 2)}{y_i! \Gamma(\phi - 2)} (1 + \phi \exp(-\xi_i))^{-y_i} (1 + \phi^{-1} \exp(\xi_i))^{-\phi}$$

where

$$\xi_i := \beta_0 + \beta_1 x_{i,1} + \ldots + \beta_p x_{i,p}.$$

Which means the probability of any realization would be

$$\mathbb{P}(Y_i = y_i) = \mathbb{P}(Y_i = 0 \mid I_i = 1) \mathbb{1}_{y_i = 0} + (1 - \mathbb{P}(Y_i = 0 \mid I_i = 1)) \mathbb{P}(Y_i = y_i \mid I_i = 0).$$

The problem is that plus sign will destroy the optimization because you can't log it effectively. Let's now consider the hurdle model.

Here, there is a probability of zero. And if it "jumps the hurdle" then we get a positive realization model. We can still model the positive realizations with a negative binomial model by just subtracting one from the counts to shift the support from $\{1, 2, ...\}$ to $\{0, 1, ...\}$. The hurdle is then defined as before where this time there is no latent "inflation" variable:

$$p_i := \mathbb{P}(Y_i = 0) := (1 + \exp(-\eta_i))^{-1}$$

 $1 - p_i = (1 + \exp(\eta_i))^{-1}$

The positive realization model is then defined as before except now we subtract one from every y_i to shift the support correctly. FROM THIS POINT ON, all $y_i \ge 1$.

$$\mathbb{P}(Y_i = y_i \mid Y_i > 0) = \begin{pmatrix} y_i + \phi - 2 \\ y_i - 1 \end{pmatrix} \left(\frac{\mu_i}{\mu_i + \phi}\right)^{y_i - 1} \left(\frac{\phi}{\mu_i + \phi}\right)^{\phi} \\
= \frac{\Gamma(y_i + \phi - 3)}{(y_i - 1)! \Gamma(\phi - 2)} \left(\frac{\mu_i}{\mu_i + \phi}\right)^{y_i - 1} \left(\frac{\phi}{\mu_i + \phi}\right)^{\phi} \\
= \frac{\Gamma(y_i + \phi - 3)}{(y_i - 1)! \Gamma(\phi - 2)} \left(\frac{\exp(\xi_i)}{\exp(\xi_i) + \phi}\right)^{y_i - 1} \left(\frac{\phi}{\exp(\xi_i) + \phi}\right)^{\phi}$$

Which means the probability of any realization would be

$$\mathbb{P}(Y_i = y_i) = \mathbb{P}(Y_i = 0) \mathbb{1}_{y_i = 0} + (1 - \mathbb{P}(Y_i = 0)) \mathbb{P}(Y_i = y_i \mid Y_i > 0) \mathbb{1}_{y_i > 0}.$$

We can make life easier by defining the augmented data $z_i := \mathbb{1}_{y_i=0}$ to obtain:

$$\mathbb{P}(Y_i = y_i, Z_i = z_i) = \mathbb{P}(Y_i = 0)^{z_i} ((1 - \mathbb{P}(Y_i = 0)) \mathbb{P}(Y_i = y_i \mid Y_i > 0))^{1 - z_i}
= p_i^{z_i} ((1 - p_i) \mathbb{P}(Y_i = y_i \mid Y_i > 0))^{1 - z_i}$$

The total likelihood function will be:

$$\mathcal{L}(\gamma_0, \gamma_1, \dots, \gamma_p, \beta_0, \beta_1, \dots, \beta_p, \phi \mid y_1, \dots, y_n, z_1, \dots, z_n)$$

$$= \prod_{i=1}^n p_i^{z_i} ((1 - p_i) \mathbb{P} (Y_i = y_i \mid Y_i > 0))^{1 - z_i}$$

And the log-likelihood will be

$$\ell(\gamma_0, \gamma_1, \ldots, \gamma_p, \beta_0, \beta_1, \ldots, \beta_p, \phi \mid y_1, \ldots, y_n, z_1, \ldots, z_n)$$

$$= \sum_{i=1}^{n} z_{i} \ln (p_{i}) + (1 - z_{i}) \ln (1 - p_{i}) + (1 - z_{i}) \ln (\mathbb{P} (Y_{i} = y_{i} \mid Y_{i} > 0))$$

$$= \sum_{i=1}^{n} z_{i} \ln ((1 + \exp(-\eta_{i}))^{-1}) + (1 - z_{i}) \ln ((1 + \exp(\eta_{i}))^{-1}) + (1 - z_{i}) \ln (\frac{\Gamma (y_{i} + \phi - 3)}{(y_{i} - 1)! \Gamma (\phi - 2)} (1 + \phi \exp(-\xi_{i}))^{-(y_{i} - 1)} (1 + \phi^{-1} \exp(\xi_{i}))^{-\phi})$$

$$= \sum_{i=1}^{n} -z_{i} \ln (1 + \exp(-\eta_{i})) - (1 - z_{i}) \ln (1 + \exp(\eta_{i})) + (1 - z_{i}) \ln (\frac{\Gamma (y_{i} + \phi - 3)}{(y_{i} - 1)! \Gamma (\phi - 2)}) + (1 - z_{i}) \ln ((1 + \phi \exp(-\xi_{i}))^{-(y_{i} - 1)}) + (1 - z_{i}) \ln ((1 + \exp(-\eta_{i})) + (1 - z_{i}) \ln (1 + \exp(\eta_{i})) + (1 - z_{i}) \ln (1 + \exp(\eta_{i})) + (1 - z_{i}) (\ln \Gamma (y_{i} + \phi - 3) - \ln \Gamma (y_{i}) - \ln \Gamma (\phi - 2)) + (y_{i} - 1)(1 - z_{i}) \ln (1 + \phi \exp(-\xi_{i})) + (0 - 2i) \ln (1 + \phi^{-1} \exp(\xi_{i}))$$

To simplify this a little bit, note that when $z_i = 1$, the summand simplifies to:

$$-\ln\left(1+\exp\left(-\eta_i\right)\right)$$

And when $z_i = 0$, the summand simplifies to:

$$-\ln(1 + \exp(\eta_i)) + (\ln\Gamma(y_i + \phi - 3) - \ln\Gamma(y_i) - \ln\Gamma(\phi - 2)) + (-(y_i - 1)\ln(1 + \phi\exp(-\xi_i)) + (-\phi\ln(1 + \phi^{-1}\exp(\xi_i)))$$

We seek to maximize this quantity over the parameters. We can start the parameters from an intelligent point by fitting a logistic regression to the z_i 's and returning a starting point for the γ_j 's. Then we can fit an OLS model to the y_i 's which are nonzero returning a starting point for the β_j 's.

When using the L-BFGS algorithm, we also need the gradient $\nabla \ell$ with respect to all of our parameters, i.e. $\gamma_0, \gamma_1, \ldots, \gamma_p, \beta_0, \beta_1, \ldots, \beta_p, \phi$. We now derive them. Assume the first column of the covariate matrix is 1. First when $z_i = 1$,

$$\frac{\partial \ell}{\partial \gamma_k} := x_{i,k} \left(1 + \exp\left(\eta_i\right) \right)^{-1}$$

and all other gradients are zero. Then when $z_i = 0$,

$$\frac{\partial \ell}{\partial \gamma_{k}} := -x_{i,k} (1 + \exp(-\eta_{i}))^{-1} - \phi (1 + \phi \exp(-\xi_{i}))^{-1}
\frac{\partial \ell}{\partial \beta_{k}} := x_{i,k} (y_{i} - 1) \phi (\phi + \exp(\xi_{i}))^{-1} - x_{i,k} \phi (1 + \phi \exp(-\xi_{i}))^{-1}
\frac{\partial \ell}{\partial \phi} := \psi(y_{i} + \phi - 3) - \psi(\phi - 2) +
-(y_{i} - 1) (\phi + \exp(\xi_{i}))^{-1} + (1 + \phi \exp(-\xi_{i}))^{-1} - \ln(\phi + \exp(\xi_{i})) + \ln(\phi)$$

where ψ denote the digamma function.