PGF operations for the Zipkin model

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1 Observation

Consider one time step. Define random variables:

- N_i = true abundance of stage i individuals
- Y_i = number of detected stage i individuals
- p_i = detection probability of stage i individuals

1.1 Unnormalized conditional PGF of N, Y = y

Let $\mathbf{y} = (y_1, y_2)$ be a vector of observations at one time step, then:

$$F_{\mathbf{N},\mathbf{Y}=\mathbf{y}}(\mathbf{s}) = \frac{1}{y_1! y_2!} (s_1 p_1)^{y_1} (s_2 p_2)^{y_2} \left[\frac{\partial^{y_1 + y_2}}{\partial u_1^{y_1} \partial u_2^{y_2}} F_{\mathbf{N}}(\mathbf{u}) \right]_{u_i = s_i (1 - p_i)}$$

Proof.

$$\begin{split} F_{\mathbf{N},\mathbf{Y}=\mathbf{y}}(\mathbf{s}) &= \frac{1}{y_1!y_2!} \left[\frac{\partial^{y_1+y_2}}{\partial t_1^{y_1} \partial t_2^{y_2}} F_{\mathbf{N},\mathbf{Y}}(\mathbf{s},\mathbf{t}) \right]_{\mathbf{t}=\mathbf{0}} \\ &= \frac{1}{y_1!y_2!} \left[\frac{\partial^{y_1+y_2}}{\partial t_1^{y_1} \partial t_2^{y_2}} F_{\mathbf{N}}(s_1(1+p_1t_1-p_1),s_2(1+p_2t_2-p_2)) \right]_{\mathbf{t}=\mathbf{0}} \\ &= \frac{1}{y_1!y_2!} \left[\left[(s_1p_1)^{y_1} (s_2p_2)^{y_2} \frac{\partial^{y_1+y_2}}{\partial u_1^{y_1} \partial u_2^{y_2}} F_{\mathbf{N}}(u_1,u_2) \right]_{u_i=s_i(1+p_it_i-p_i)} \right]_{\mathbf{t}=\mathbf{0}} \\ &= \frac{1}{y_1!y_2!} (s_1p_1)^{y_1} (s_2p_2)^{y_2} \left[\frac{\partial^{y_1+y_2}}{\partial u_1^{y_1} \partial u_2^{y_2}} F_{\mathbf{N}}(u_1,u_2) \right]_{u_i=s_i(1-p_i)} \end{split}$$

1.2 Invariance of the functional form

Suppose $F_{\mathbf{N}}(\mathbf{u}) = f(\mathbf{u})e^{\mathbf{a}^T\mathbf{u}+a_0}$, where $f(\mathbf{u})$ is a bivariate polynomial of degree d. Then, after observing evidence, the PGF maintains the same form $F_{\mathbf{N},\mathbf{Y}=\mathbf{y}}(\mathbf{s}) = g(\mathbf{s})e^{\mathbf{b}^T\mathbf{s}+b_0}$, where $g(\mathbf{s})$ is a bivariate polynomial of degree $d+y_1+y_2$.

Proof.

$$\begin{split} F_{\mathbf{N},\mathbf{Y}=\mathbf{y}}(\mathbf{s}) &= \frac{1}{y_1!y_2!} (s_1p_1)^{y_1} (s_2p_2)^{y_2} \left[\frac{\partial^{y_1+y_2}}{\partial u_1^{y_1} \partial u_2^{y_2}} F_{\mathbf{N}}(u_1, u_2) \right]_{u_i = s_i(1-p_i)} \\ &= \frac{1}{y_1!y_2!} (s_1p_1)^{y_1} (s_2p_2)^{y_2} \left[\frac{\partial^{y_1+y_2}}{\partial u_1^{y_1} \partial u_2^{y_2}} f(\mathbf{u}) e^{\mathbf{a}^T \mathbf{u} + a_0} \right]_{u_i = s_i(1-p_i)} \\ &= \frac{1}{y_1!y_2!} (s_1p_1)^{y_1} (s_2p_2)^{y_2} \left[e^{\mathbf{a}^T \mathbf{u} + a_0} \sum_{l=0}^{y_1} \binom{y_1}{l} a_1^{y_1-l} \sum_{m=0}^{y_2} \binom{y_2}{m} a_2^{y_2-m} \right. \\ &\left. \frac{\partial^{l+m}}{\partial u_1^l \partial u_2^m} f(u_1, u_2) \right]_{u_i = s_i(1-p_i)} \\ &= \frac{1}{y_1!y_2!} (s_1p_1)^{y_1} (s_2p_2)^{y_2} e^{a_1s_1(1-p_1) + a_2s_2(1-p_2) + a_0} \sum_{l=0}^{y_1} \frac{y_1!}{l!(y_1-l)!} a_1^{y_1} a_1^{-l} \\ &\sum_{m=0}^{y_2} \frac{y_2!}{m!(y_2-m)!} a_2^{y_2} a_2^{-m} f_{u_1^l u_2^m} (s_1(1-p_1), s_2(1-p_2)) \\ &= e^{a_1(1-p_1)s_1 + a_2(1-p_2)s_2 + a_0} \sum_{l=0}^{y_1} \sum_{m=0}^{y_2} \frac{(a_1p_1)^{y_1}}{l!(y_1-l)!} \frac{(a_2p_2)^{y_2}}{m!(y_2-m)!a_2^m} \\ &s_1^{y_1} s_2^{y_2} f_{u_1^l u_2^m} (s_1(1-p_1), s_2(1-p_2)) \end{split}$$

The first term has the form $e^{\mathbf{b}^T\mathbf{s}+b_0}$, where $\mathbf{b}=(a_1(1-p_1),a_2(1-p_2))$ and $b_0=a_0$. Since the mixed partial derivative of a bivariate polynomial of degree d is also a bivariate polynomial of degree at most d, and the scalar $\frac{(a_1p_1)^{y_1}}{l!(y_1-l)!a_1^l}\frac{(a_2p_2)^{y_2}}{m!(y_2-m)!a_2^m}$ can be combined with the coefficient of each monomial of $f_{u_1^lu_2^m}(s_1(1-p_1),s_2(1-p_2))$, the term inside the summation is a bivariate polynomial of degree at most $d+y_1+y_2$. Furthermore, since the sum of polynomials is another polynomial of the same degree as its highest-degree term, the entire summation term must be a bivariate polynomial of degree $d+y_1+y_2$.

2 Transition

2.1 PGF of a multinomial rv

If $\mathbf{Z}|N \sim Multinomial(N, \mathbf{p})$, then $F_{\mathbf{Z}|N}(\mathbf{t}) = (\sum_k t_k p_k)^N$.

Proof.

$$\begin{split} F_{\mathbf{Z}|N}(\mathbf{t}) &= E_{\mathbf{Z}|N}(\prod_k t_k^{Z_k}|N) \\ &= \sum_{\mathbf{z}} \prod_k t_k^{z_k} p(\mathbf{z}|n) \\ &= \sum_{\mathbf{z}} \prod_k t_k^{z_k} \frac{n!}{\prod_k z_k!} \prod_k p_k^{z_k} \\ &= \sum_{\mathbf{z}} \frac{n!}{\prod_k z_k!} \prod_k (t_k p_k)^{z_k} \\ &= (\sum_k t_k p_k)^n, \text{ by the multinomial theorem} \end{split}$$

2.2 Joint PGF over $\{Z_{ij}\}$

If $\mathbf{Z}_1|N_1 \sim Multinomial(N_1, \mathbf{p}_1)$ and $\mathbf{Z}_2|N_2 \sim Multinomial(N_2, \mathbf{p}_2)$, then $F_{\mathbf{Z}_1,\mathbf{Z}_2}(\mathbf{t}_1,\mathbf{t}_2) = F_{\mathbf{N}_1,\mathbf{N}_2}(\sum_j t_{1j}p_{1j},\sum_j t_{2j}p_{2j})$.

Proof. First, find $F_{\mathbf{Z}_1,\mathbf{Z}_2|N_1,N_2}(\mathbf{t}_1,\mathbf{t}_2)$:

$$\begin{split} F_{\mathbf{Z}_{1},\mathbf{Z}_{2}|N_{1},N_{2}}(\mathbf{t}_{1},\mathbf{t}_{2}) &= \sum_{\mathbf{z}_{1},\mathbf{z}_{2}} \prod_{ij} t_{ij}^{z_{ij}} p(\mathbf{z}_{1},\mathbf{z}_{2}|n_{1},n_{2}) \\ &= \sum_{\mathbf{z}_{1},\mathbf{z}_{2}} \prod_{ij} t_{ij}^{z_{ij}} p(\mathbf{z}_{1}|n_{1}) p(\mathbf{z}_{2}|n_{2}) \\ &= \sum_{\mathbf{z}_{1}} \prod_{j} t_{1j}^{z_{1j}} p(\mathbf{z}_{1}|n_{1}) \sum_{\mathbf{z}_{2}} \prod_{j} t_{2j}^{z_{2j}} p(\mathbf{z}_{2}|n_{2}) \\ &= (\sum_{i} t_{1j} p_{1j})^{n_{1}} (\sum_{i} t_{2j} p_{2j})^{n_{2}} \end{split}$$

Find the joint PGF over $\mathbf{Z}_1, \mathbf{Z}_2, N_1, N_2$:

$$\begin{split} F_{N_1,N_2,\mathbf{Z}_1,\mathbf{Z}_2}(s_1,s_2,\mathbf{t}_1,\mathbf{t}_2) &= \sum_{n_1,n_2,\mathbf{z}_1,\mathbf{z}_2} \prod_i s_i^{n_i} \prod_j t_{ij}^{z_{ij}} p(n_1,n_2,\mathbf{z}_1,\mathbf{z}_2) \\ &= \sum_{n_1,n_2,\mathbf{z}_1,\mathbf{z}_2} \prod_i s_i^{n_i} \prod_j t_{ij}^{z_{ij}} p(\mathbf{z}_1,\mathbf{z}_2|n_1,n_2) p(n_1,n_2) \\ &= \sum_{n_1,n_2} \prod_i s_i^{n_i} p(n_1,n_2) \sum_{\mathbf{z}_1,\mathbf{z}_2} \prod_i t_{ij}^{z_{ij}} p(\mathbf{z}_1,\mathbf{z}_2|n_1,n_2) \\ &= \sum_{n_1,n_2} \prod_i s_i^{n_i} p(n_1,n_2) (\sum_j t_{1j} p_{1j})^{n_1} (\sum_j t_{2j} p_{2j})^{n_2} \\ &= \sum_{n_1,n_2} \prod_i (s_i \sum_j t_{ij} p_{ij})^{n_i} p(n_1,n_2) \\ &= F_{N_1,N_2}(s_1 \sum_j t_{1j} p_{1j},s_2 \sum_j t_{2j} p_{2j}) \end{split}$$

Finally, marginalize to obtain:

$$\begin{split} F_{\mathbf{Z}_1,\mathbf{Z}_2}(\mathbf{t}_1,\mathbf{t}_2) &= F_{N_1,N_2,\mathbf{Z}_1,\mathbf{Z}_2}(1,1,\mathbf{t}_1,\mathbf{t}_2) \\ &= F_{N_1,N_2}(\sum_j t_{1j}p_{1j},\sum_j t_{2j}p_{2j}) \end{split}$$

2.3 Joint PGF over M_1, M_2

If $m_1 = z_{11} + z_{21}$ and $m_2 = z_{12} + z_{22}$, then $F_{M_1, M_2}(u_1, u_2) = F_{N_1, N_2}(\sum_j u_j p_{1j}, \sum_j u_j p_{2j})$ Proof. Since $m_j = z_{1j} + z_{2j}$:

$$F_{M_j|Z_{1j},Z_{2j}}(u_j) = \sum_{m_j} u_j^{m_j} p(m_j|z_{1j},z_{2j})$$
$$= u_j^{z_{1j}+z_{2j}}$$

Find the conditional PGF:

$$\begin{split} F_{M_1,M_2|\mathbf{Z}_1,\mathbf{Z}_2}(u_1,u_2) &= \sum_{m_1,m_2} \prod_j u_j^{m_j} p(m_1,m_2|\mathbf{z}_1,\mathbf{z}_2) \\ &= \sum_{m_1,m_2} \prod_j u_j^{m_j} p(m_1|z_{11},z21) p(m_2|z_{12},z_{22}) \\ &= \sum_{m_1} u_1^{m_1} p(m_1|z_{11},z21) \sum_{m_2} u_2^{m_2} p(m_2|z_{12},z_{22}) \\ &= \prod_j u_j^{z_{1j}+z_{2j}} \end{split}$$

Then the joint PGF:

$$\begin{split} F_{\mathbf{Z}_1,\mathbf{Z}_2,M_1,M_2}(\mathbf{t}_1,\mathbf{t}_2,u_1,u_2) &= \sum_{\mathbf{z}_1,\mathbf{z}_2,m_1,m_2} \prod_i u_i^{m_i} \prod_j t_{ij}^{z_{ij}} p(\mathbf{z}_1,\mathbf{z}_2,m_1,m_2) \\ &= \sum_{\mathbf{z}_1,\mathbf{z}_2,m_1,m_2} \prod_i u_i^{m_i} \prod_j t_{ij}^{z_{ij}} p(m_1,m_2|\mathbf{z}_1,\mathbf{z}_2) p(\mathbf{z}_1,\mathbf{z}_2) \\ &= \sum_{\mathbf{z}_1,\mathbf{z}_2} \prod_{ij} t_{ij}^{z_{ij}} p(\mathbf{z}_1,\mathbf{z}_2) \sum_{m_1,m_2} \prod_i u_i^{m_i} p(m_1,m_2|\mathbf{z}_1,\mathbf{z}_2) \\ &= \sum_{\mathbf{z}_1,\mathbf{z}_2} \prod_{ij} t_{ij}^{z_{ij}} p(\mathbf{z}_1,\mathbf{z}_2) \prod_j u_j^{z_{1j}+z_{2j}} \\ &= \sum_{\mathbf{z}_1,\mathbf{z}_2} \prod_{ij} (u_j t_{ij})^{z_{ij}} p(\mathbf{z}_1,\mathbf{z}_2) \\ &= F_{\mathbf{Z}_1,\mathbf{Z}_2}(u_1 t_{11},u_2 t_{12},u_1 t_{21},u_2 t_{22}) \\ &= F_{N_1,N_2}(u_1 t_{11} p11 + u_2 t_{12} p_{12},u_1 t_{21} p21 + u_2 t_{22} p_{22}) \end{split}$$

So the marginal PGF over M_1, M_2 is:

$$\begin{split} F_{M_1,M_2}(u_1,u_2) &= F_{1,1,M_1,M_2}(\mathbf{t}_1,\mathbf{t}_2,u_1,u_2) \\ &= F_{N_1,N_2}(u_1p11 + u_2p_{12},u_1p21 + u_2p_{22}) \end{split}$$

Therefore, $F_{\mathbf{M}}(\mathbf{u}) = F_{\mathbf{N}}(\mathbf{P}\mathbf{u}).$

2.4 Invariance of the functional form

Suppose $F_{\mathbf{N},\mathbf{Y}(\mathbf{u})=\mathbf{y}}(\mathbf{s}) = f(\mathbf{u})e^{\mathbf{a}^T\mathbf{u}+a_0}$, where $f(\mathbf{u})$ is a bivariate polynomial of degree d. Then, after the transition operation, the PGF still has the same form $F_{\mathbf{N}}(\mathbf{s}) = g(\mathbf{s})e^{\mathbf{b}^T\mathbf{s}+b_0}$, where $g(\mathbf{s})$ is also a bivariate polynomial of degree d.

Proof.

$$F_{\mathbf{N}}(\mathbf{s}) = F_{\mathbf{N},\mathbf{Y}}(\Delta \mathbf{s})$$

$$= f(\Delta \mathbf{s})e^{\mathbf{a}^T \Delta \mathbf{s} + a_0}$$

$$= g(\mathbf{s})e^{(\mathbf{a}^T \Delta)\mathbf{s} + a_0}$$

Let $h(\mathbf{s}) = \Delta \mathbf{s}$, then the first term is the composition of a bivariate polynomial of degree d and a linear transformation of a vector, $g(\mathbf{s}) = foh(\mathbf{s})$, which is another bivariate polynomial of degree d by ???. The second term has the form $e^{\mathbf{b}^T \mathbf{s} + b_0}$, where $\mathbf{b}^T = \mathbf{a}^T \Delta$ and $b_0 = a_0$.

3 Reproduction

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