PGF operations for the Zipkin model

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1 Observation

Consider one time step. Define:

- N_i: true abundance of stage i individuals
- Y_i: observed abundance of stage i individuals
- P_i: detection probability of stage i individuals

1.1 Unnormalized conditional PGF of $\mathbf{N}$, $\mathbf{Y} = \mathbf{y}$

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

$$F_{\mathbf{N},\mathbf{Y}=\mathbf{y}}(\mathbf{s}) = \frac{1}{y_1!y_2!}(s_1p_1)^{y_1}(s_2p_2)^{y_2}\left[\frac{\partial^{y_1+y_2}}{\partial u_1^{y_1}\partial u_2^{y_2}}F_{\mathbf{N}}(\mathbf{u})\right]_{u_i=s_i(1-p_i)}$$

Proof.

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

□

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.

$$
\begin{aligned}
F_{\mathbf{N},\mathbf{Y}=\mathbf{y}}(\mathbf{s}) &= \frac{1}{y_1!y_2!}(s_1p_1)^{y_1}(s_2p_2)^{y_2}\left[\frac{\partial^{y_1+y_2}}{\partial u_1^{y_1}\partial u_2^{y_2}}F_{\mathbf{N}}(u_1,u_2)\right]_{u_i=s_i(1-p_i)} \\
&= \frac{1}{y_1!y_2!}(s_1p_1)^{y_1}(s_2p_2)^{y_2}\left[\frac{\partial^{y_1+y_2}}{\partial u_1^{y_1}\partial u_2^{y_2}}f(\mathbf{u})e^{\mathbf{a}^T\mathbf{u}+a_0}\right]_{u_i=s_i(1-p_i)} \\
&= \frac{1}{y_1!y_2!}(s_1p_1)^{y_1}(s_2p_2)^{y_2}\left[e^{\mathbf{a}^T\mathbf{u}+a_0}\sum_{l=0}^{y_1}\binom{y_1}{l}a_1^{y_1-l}\sum_{m=0}^{y_2}\binom{y_2}{m}a_2^{y_2-m}\right. \\
&\quad \left.\frac{\partial^{l+m}}{\partial u_1^l\partial u_2^m}f(u_1,u_2)\right]_{u_i=s_i(1-p_i)} \\
&= \frac{1}{y_1!y_2!}(s_1p_1)^{y_1}(s_2p_2)^{y_2}e^{a_1s_1(1-p_1)+a_2s_2(1-p_2)+a_0}\sum_{l=0}^{y_1}\frac{y_1!}{l!(y_1-l)!}a_1^{y_1}a_1^{-l} \\
&\quad \sum_{m=0}^{y_2}\frac{y_2!}{m!(y_2-m)!}a_2^{y_2}a_2^{-m}f_{u_1^lu_2^m}(s_1(1-p_1),s_2(1-p_2)) \\
&= e^{a_1(1-p_1)s_1+a_2(1-p_2)s_2+a_0}\sum_{l=0}^{y_1}\sum_{m=0}^{y_2}\frac{(a_1p_1)^{y_1}(a_2p_2)^{y_2}}{l!m!(y_1-l)!(y_2-m)!a_1^la_2^m} \\
&\quad s_1^{y_1}s_2^{y_2}f_{u_1^lu_2^m}(s_1(1-p_1),s_2(1-p_2))
\end{aligned}
$$

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 $\frac{(a_1p_1)^{y_1}(a_2p_2)^{y_2}}{l!m!(y_1-l)!(y_2-m)!a_1^la_2^m}$ 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

Define:

- N_i: true abundance of stage i individuals at the previous time step
- Z_{ij}: number of stage i individuals that transition to stage j
- P_{ij}: transition probability from i to j
- $M_i = Z_{1i}+Z_{2i}$: abundance of stage i individuals at the current time step after the transition operation

2.1 PGF of a multinomial random variable

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

Proof.

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

□

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

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

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

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

Finally, marginalize to obtain:

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

□

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 $m_j = z_{1j} + z_{2j}$:

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

Find the conditional PGF:

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

Then the joint PGF:

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

So the marginal PGF over M_1, M_2 is:

$$\begin{aligned}
F_{M_1,M_2}(u_1,u_2) &= F_{1,1,M_1,M_2}(\mathbf{t}_1,\mathbf{t}_2,u_1,u_2) \\
&= F_{N_1,N_2}(u_1 p11 + u_2 p_{12}, u_1 p21 + u_2 p_{22})
\end{aligned}$$

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

□

2.4 Composition of a multivariate polynomial and a linear transformation

If $f(\mathbf{u})$ is a polynomial of n variables of degree d and $g(\mathbf{s})$ is a linear transformation $g : \mathbb{R}^m \mapsto \mathbb{R}^n$, then the composition $f \circ g(\mathbf{s})$ is a polynomial of m variables of degree d.

Proof. Suppose $f(\mathbf{u}) = \sum_{k_1=0}^{d_1} \ldots \sum_{k_n=0}^{d_n} c_{\mathbf{k}} u_1^{k_1} \ldots u_n^{k_n}$, where $d = d_1 + \ldots + d_n$. Furthermore, suppose $g(\mathbf{s}) = \mathbf{As} + \mathbf{b}$, where $\mathbf{A} \in \mathbb{R}^{m \times n}$, $\mathbf{s} \in \mathbb{R}^m$, and $\mathbf{b} \in \mathbb{R}^n$. Then the composition of f and g:

$$
\begin{aligned}
f \circ g(\mathbf{s}) &= f(g(\mathbf{s})) \\
&= \sum_{k_1=0}^{d_1} \ldots \sum_{k_n=0}^{d_n} c_{\mathbf{k}} (A_{11}s_1 + \ldots + A_{1m}s_m + b_1)^{k_1} \ldots (A_{n1}s_1 + \ldots + A_{nm}s_m + b_n)^{k_n} \\
&= \sum_{\mathbf{k}} c_{\mathbf{k}} \sum_{\mathbf{l}_1 : \sum_j l_{1j} = k_1} \frac{k_1!}{l_{11}! \ldots l_{1m}! l_{1m+1}!} (A_{11}s_1)^{l_{11}} \ldots (A_{1m}s_m)^{l_{1m}} b_1^{l_{1m+1}} \ldots \\
&\quad \sum_{\mathbf{l}_n : \sum_j l_{1j} = k_n} \frac{k_n!}{l_{n1}! \ldots l_{nm}! l_{nm+1}!} (A_{n1}s_1)^{l_{n1}} \ldots (A_{nm}s_m)^{l_{nm}} b_n^{l_{nm+1}} \\
&= \sum_{\mathbf{k}} c_{\mathbf{k}} \sum_{\mathbf{l}_1 : \sum_j l_{1j} = k_1} \frac{k_1!}{l_{11}! \ldots l_{1m}! l_{1m+1}!} A_{11}^{l_{11}} \ldots A_{1m}^{l_{1m}} b_1^{l_{1m+1}} \ldots \\
&\quad \sum_{\mathbf{l}_n : \sum_j l_{1j} = k_n} \frac{k_n!}{l_{n1}! \ldots l_{nm}! l_{nm+1}!} A_{n1}^{l_{n1}} \ldots A_{nm}^{l_{nm}} b_n^{l_{nm+1}} s_1^{\sum_i l_{i1}} \ldots s_m^{\sum_i l_{im}}
\end{aligned}
$$

which is a polynomial of m variables. The degree of this polynomial is:

$$
\begin{aligned}
\sum_i \max(l_{i1}) + \ldots + \sum_i \max(l_{im}) &= \sum_j \max(l_{1j}) + \ldots + \sum_j \max(l_{nj}) \\
&= d_1 + \ldots + d_n \\
&= d
\end{aligned}
$$

Therefore, $f \circ g(\mathbf{s})$ is a polynomial of m variables of degree d.

□

2.5 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 the transition operation, the PGF still has the same form $F_{\mathbf{M}}(\mathbf{s}) = g(\mathbf{s})e^{\mathbf{b}^T\mathbf{s}+b_0}$, where $g(\mathbf{s})$ is also a bivariate polynomial of degree d.

Proof.

$$
\begin{aligned}
F_{\mathbf{M}}(\mathbf{s}) &= F_{\mathbf{N}}(\mathbf{Ps}) \\
&= f(\mathbf{Ps})e^{\mathbf{a}^T(\mathbf{Ps})+a_0} \\
&= g(\mathbf{s})e^{(\mathbf{a}^T\mathbf{P})\mathbf{s}+a_0}
\end{aligned}
$$

The first term, $g(\mathbf{s}) = f \circ h(\mathbf{s})$, is a composition of a bivariate polynomial of degree d and a linear transformation $h(\mathbf{s}) = \mathbf{Ps}$, which is another bivariate polynomial of degree d by section 2.4. The second term has the form $e^{\mathbf{b}^T\mathbf{s}+b_0}$, where $\mathbf{b}^T = \mathbf{a}^T\mathbf{P}$ and $b_0 = a_0$.

□

3 Reproduction