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
- D: total number of stages

1.1 Multivariate evidence

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

$$F_{\mathbf{N},\mathbf{Y}=\mathbf{y}}(\mathbf{s}) = \frac{1}{\prod_d y_d!}\left[\frac{\partial^{y_1+\ldots+y_D}}{\partial t_1^{y_1}\ldots\partial t_D^{y_D}} F_{\mathbf{N},\mathbf{Y}}(\mathbf{s},\mathbf{t})\right]_{\mathbf{t}=\mathbf{0}}$$

Proof.

$$\begin{aligned}
&\frac{1}{\prod_d y_d!}\left[\frac{\partial^{y_1+\ldots+y_D}}{\partial t_1^{y_1}\ldots\partial t_D^{y_D}} F_{\mathbf{N},\mathbf{Y}}(\mathbf{s},\mathbf{t})\right]_{\mathbf{t}=\mathbf{0}} \\
&\quad= \frac{1}{\prod_d y_d!}\left[\frac{\partial^{y_1+\ldots+y_D}}{\partial t_1^{y_1}\ldots\partial t_D^{y_D}} \sum_{\mathbf{n},\mathbf{y}'}\prod_d s_d^{n_d} t_d^{y_d} p(\mathbf{n},\mathbf{y}')\right]_{\mathbf{t}=\mathbf{0}} \\
&\quad= \frac{1}{\prod_d y_d!}\sum_{\mathbf{n}}\prod_d s_d^{n_d}\sum_{\mathbf{y}'} p(\mathbf{n},\mathbf{y}')\left[\frac{\partial^{y_1+\ldots+y_D}}{\partial t_1^{y_1}\ldots\partial t_D^{y_D}}\prod_d t_d^{y_d}\right]_{\mathbf{t}=\mathbf{0}} \\
&\quad= \frac{1}{\prod_d y_d!}\sum_{\mathbf{n}}\prod_d s_d^{n_d} p(\mathbf{n},\mathbf{y})\prod_d y_d! \\
&\quad= F_{\mathbf{N},\mathbf{Y}=\mathbf{y}}(\mathbf{s})
\end{aligned}$$

□

1.2 Thin then observe multiple variables

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

$$F_{\mathbf{N},\mathbf{Y}=\mathbf{y}}(\mathbf{s}) = \frac{1}{\prod_d y_d!} \prod_d (s_d p_d)^{y_d} \left[\frac{\partial^{y_1+\ldots+y_D}}{\partial u_1^{y_1} \ldots \partial u_D^{y_D}} F_{\mathbf{N}}(\mathbf{u}) \right]_{u_i = s_i(1-p_i)}$$

Proof.

$$\begin{aligned}
F_{\mathbf{N},\mathbf{Y}=\mathbf{y}}(\mathbf{s}) &= \frac{1}{\prod_d y_d!} \left[\frac{\partial^{y_1+\ldots+y_D}}{\partial t_1^{y_1} \ldots \partial t_D^{y_D}} F_{\mathbf{N},\mathbf{Y}}(\mathbf{s}, \mathbf{t}) \right]_{\mathbf{t}=\mathbf{0}} \\
&= \frac{1}{\prod_d y_d!} \left[\frac{\partial^{y_1+\ldots+y_D}}{\partial t_1^{y_1} \ldots \partial t_D^{y_D}} F_{\mathbf{N}}(s_1(1+p_1 t_1 - p_1), \ldots, s_D(1+p_D t_D - p_D)) \right]_{\mathbf{t}=\mathbf{0}} \\
&= \frac{1}{\prod_d y_d!} \left[\left[\prod_d (s_d p_d)^{y_d} \frac{\partial^{y_1+\ldots+y_D}}{\partial u_1^{y_1} \ldots \partial u_D^{y_D}} F_{\mathbf{N}}(\mathbf{u}) \right]_{u_i = s_i(1+p_i t_i - p_i)} \right]_{\mathbf{t}=\mathbf{0}} \\
&= \frac{1}{\prod_d y_d!} \prod_d (s_d p_d)^{y_d} \left[\frac{\partial^{y_1+\ldots+y_D}}{\partial u_1^{y_1} \ldots \partial u_D^{y_D}} F_{\mathbf{N}}(\mathbf{u}) \right]_{u_i = s_i(1-p_i)}
\end{aligned}$$

□

1.3 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 polynomial of n variables 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 polynomial of n variables of degree $d + y_1 + \ldots + y_D$.

Proof.

$$\begin{aligned}
F_{\mathbf{N},\mathbf{Y}=\mathbf{y}}(\mathbf{s}) &= \frac{1}{\prod_d y_d!} \prod_d (s_d p_d)^{y_d} \left[\frac{\partial^{y_1+\ldots+y_D}}{\partial u_1^{y_1} \ldots \partial u_D^{y_D}} F_{\mathbf{N}}(\mathbf{u}) \right]_{u_i = s_i(1-p_i)} \\
&= \frac{1}{\prod_d y_d!} \prod_d (s_d p_d)^{y_d} \left[\frac{\partial^{y_1+\ldots+y_D}}{\partial u_1^{y_1} \ldots \partial u_D^{y_D}} f(\mathbf{u}) e^{\mathbf{a}^T \mathbf{u} + a_0} \right]_{u_i = s_i(1-p_i)} \\
&= \frac{1}{\prod_d y_d!} \prod_d (s_d p_d)^{y_d} \left[e^{\mathbf{a}^T \mathbf{u} + a_0} \sum_{l_1=0}^{y_1} \cdots \sum_{l_D=0}^{y_D} \prod_d \binom{y_d}{l_d} a_d^{y_d - l_d} \right. \\
&\quad \left. \frac{\partial^{l_1+\ldots+l_D}}{\partial u_1^{l_1} \ldots \partial u_D^{l_D}} f(\mathbf{u}) \right]_{u_i = s_i(1-p_i)} \\
&= \frac{1}{\prod_d y_d!} \prod_d (s_d p_d)^{y_d} e^{a_1 s_1 (1-p_1) + \ldots + a_D s_D (1-p_D) + a_0} \\
&\quad \sum_{\mathbf{l}} \prod_d \frac{y_d!}{l_d! (y_d - l_d)!} a_d^{y_d - l_d} \left[\frac{\partial^{l_1+\ldots+l_D}}{\partial u_1^{l_1} \ldots \partial u_D^{l_D}} f(\mathbf{u}) \right]_{u_i = s_i(1-p_i)} \\
&= e^{\mathbf{b}^T \mathbf{s} + b_0} \sum_{\mathbf{l}} \prod_d \frac{(a_d p_d)^{y_d}}{l_d! (y_d - l_d)! a_d^{l_d}} s_d^{y_d} \left[\frac{\partial^{l_1+\ldots+l_D}}{\partial u_1^{l_1} \ldots \partial u_D^{l_D}} f(\mathbf{u}) \right]_{u_i = s_i(1-p_i)}
\end{aligned}$$

where $\mathbf{b} = [a_d(1-p_d)]_{d=1}^D$ and $b_0 = a_0$.

Line 3 uses the product rule for mixed partial derivatives [1]. Since the mixed partial derivative of a polynomial of n variables of degree d is also a polynomial of n variables of degree at most d, and the scalar $\prod_d \frac{(a_d p_d)^{y_d}}{l_d!(y_d-l_d)!a_d^{l_d}}$ can be combined with the coefficient of each monomial of the mixed partial derivative, the term inside the summation is a polynomial of n variables of degree at most $d+\sum_i y_i$. 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 polynomial of n variables of degree $d+\sum_i y_i$.

□

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:

$$\begin{aligned}
F_{\mathbf{Z}_1,\mathbf{Z}_2,M_1,M_2}(\mathbf{t}_1, \mathbf{t}_2, u_1, u_2) &= \sum_{\mathbf{z}_1,\mathbf{z}_2,m_1,m_2} \prod_i u_i^{m_i} \prod_j t_{ij}^{z_{ij}} p(\mathbf{z}_1, \mathbf{z}_2, m_1, m_2) \\
&= \sum_{\mathbf{z}_1,\mathbf{z}_2,m_1,m_2} \prod_i u_i^{m_i} \prod_j t_{ij}^{z_{ij}} p(m_1, m_2|\mathbf{z}_1, \mathbf{z}_2)p(\mathbf{z}_1, \mathbf{z}_2) \\
&= \sum_{\mathbf{z}_1,\mathbf{z}_2} \prod_{ij} t_{ij}^{z_{ij}} p(\mathbf{z}_1, \mathbf{z}_2) \sum_{m_1,m_2} \prod_i u_i^{m_i} p(m_1, m_2|\mathbf{z}_1, \mathbf{z}_2) \\
&= \sum_{\mathbf{z}_1,\mathbf{z}_2} \prod_{ij} t_{ij}^{z_{ij}} p(\mathbf{z}_1, \mathbf{z}_2) \prod_j u_j^{z_{1j}+z_{2j}} \\
&= \sum_{\mathbf{z}_1,\mathbf{z}_2} \prod_{ij} (u_j t_{ij})^{z_{ij}} p(\mathbf{z}_1, \mathbf{z}_2) \\
&= F_{\mathbf{Z}_1,\mathbf{Z}_2}(u_1t_{11}, u_2t_{12}, u_1t_{21}, u_2t_{22}) \\
&= F_{N_1,N_2}(u_1t_{11}p11 + u_2t_{12}p_{12}, u_1t_{21}p21 + u_2t_{22}p_{22})
\end{aligned}$$

So the marginal PGF over M_1, M_2 is:

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

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

$\square$

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 $f(\mathbf{u}) = \sum_{k_1=0}^{d_1} \dots \sum_{k_n=0}^{d_n} c_{\mathbf{k}} u_1^{k_1} \dots u_n^{k_n}$, where $d = d_1 + \dots + d_n$. Furthermore, suppose $g(\mathbf{s}) = \mathbf{A}\mathbf{s} + \mathbf{b}$, 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:

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

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

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

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.

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

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 $h(\mathbf{s}) = \mathbf{P}\mathbf{s}$, 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 $b_0 = a_0$.

$\square$

3 Reproduction

Univariate case.

$$X_i = \begin{cases} 0 & \text{dies} \\ 1 & \text{survives} \\ 2 & \text{survives with 1 offspring} \end{cases}$$

Let $P(X_i = x_i) = p_{x_i}$ and $R = \sum_i^N X_i$. The PGF of X_i is given by $F_{X_i}(v) = p_0 + p_1 v + p_2 v^2$, therefore:

$$F_R(v) = F_N(F_{X_i}(v)) = F_N(p_0 + p_1 v + p_2 v^2)$$

.

3.1 Invariance of the functional form

All PGFs will have the form $e^{f_1(s)} f_2(s)$, where $f_1(s)$ is a polynomial of degree at most 2^K and $f_2(s)$ is a polynomial of degree at most $2^K \sum_k y_k$.

3.1.1 Observation

Suppose $F_N(u) = e^{f_1(u)} f_2(u)$, where $f_i(u)$ is a polynomial of degree d_i. Then $F_{N,Y=y}(s) = e^{g_1(s)} g_2(s)$, where $g_1(s)$ is a polynomial of degree d_1 and $g_2(s)$ is a polynomial of degree $yd_1 + d_2$.

3.1.2 Reproduction

Suppose $F_N(u) = e^{f_1(u)} f_2(u)$, where $f_i(u)$ is a polynomial of degree d_i. Let R be the abundance after the reproduction operation. Then $F_R(s) = e^{g_1(s)} g_2(s)$, where $g_i(s)$ is a polynomial of degree $2d_i$.

3.1.3 Arrival

Suppose $F_R(u) = e^{f_1(u)} f_2(u)$, where $f_i(u)$ is a polynomial of degree d_i. Let N be the abundance after new arrival. Then $F_N(s) = e^{g_1(s)} g_2(s)$, where $g_i(s)$ is a polynomial of degree d_i.

References

[1] Michael Hardy. Combinatorics of partial derivatives. *Electron. J. Combin*, 13(1):13, 2006.