

A Proofs — Operations on Generating Functions

Proof of Proposition 1. This is a standard fact about multivariate PGFs:

$$F_\alpha(s_{\alpha \setminus i}, 1) = \sum_{x_\alpha} \psi_\alpha(x_\alpha) s_{\alpha \setminus i}^{x_{\alpha \setminus i}} 1^{x_i} = \sum_{x_{\alpha \setminus i}} \left(\sum_{x_i} \psi_\alpha(x_{\alpha \setminus i}, x_i) \right) s_{\alpha \setminus i}^{x_{\alpha \setminus i}}$$

The fact $\sum_{x_\alpha} \psi_\alpha(x_\alpha) = F_\alpha(1, \dots, 1)$ follows by marginalizing each variable one at a time. \square

Proof of Proposition 2.

$$\frac{\partial^a}{\partial s_i^a} F_\alpha(s_\alpha) \Big|_{s_i=0} = \sum_{x_{\alpha \setminus i}} \sum_{x_i} \psi_\alpha(x_{\alpha \setminus i}, x_i) s_{\alpha \setminus i}^{x_{\alpha \setminus i}} \frac{\partial^a}{\partial s_i^a} s_i^{x_i} \Big|_{s_i=0} = a! \sum_{x_{\alpha \setminus i}} \psi_\alpha(x_{\alpha \setminus i}, a) s_{\alpha \setminus i}^{x_{\alpha \setminus i}}$$

The final equality holds because $\frac{\partial^a}{\partial s_i^a} s_i^{x_i} \Big|_{s_i=0} = a!$ if $x_i = a$ and zero otherwise. \square

Proof of Proposition 3. The PGF is

$$\begin{aligned} F_{\alpha \cup j}(s_\alpha, s_j) &= \sum_{x_\alpha} \sum_{x_j} \psi_\alpha(x_\alpha) \text{Binomial}(x_j | x_i, \rho) s_\alpha^{x_\alpha} s_j^{x_j} \\ &= \sum_{x_\alpha} \psi_\alpha(x_\alpha) s_\alpha^{x_\alpha} \sum_{x_j} \text{Binomial}(x_j | x_i, \rho) s_j^{x_j} \\ &= \sum_{x_\alpha} \psi_\alpha(x_\alpha) s_\alpha^{x_\alpha} (\rho s_j + 1 - \rho)^{x_i} \\ &= \sum_{x_\alpha} \psi_\alpha(x_\alpha) s_{\alpha \setminus i}^{x_{\alpha \setminus i}} (s_i(\rho s_j + 1 - \rho))^{x_i} \\ &= F_\alpha(s_{\alpha \setminus i}, s_i(\rho s_j + 1 - \rho)) \end{aligned}$$

In the third line, we used the fact that the PGF of the Binomial distribution is $\sum_x \text{Binomial}(x|n, \rho) s^x = (\rho s + 1 - \rho)^n$. \square

Proof of Proposition 4.

$$\begin{aligned} F_\gamma(s_\alpha, s_\beta, s_k) &= \sum_{x_\alpha, x_\beta, x_k} \psi_\alpha(x_\alpha) \psi_\beta(x_\beta) \mathbb{I}\{x_k = x_i + x_j\} s_\alpha^{x_\alpha} s_\beta^{x_\beta} s_k^{x_k} \\ &= \sum_{x_\alpha, x_\beta} \psi_\alpha(x_\alpha) \psi_\beta(x_\beta) s_\alpha^{x_\alpha} s_\beta^{x_\beta} s_k^{x_i + x_j} \\ &= \sum_{x_\alpha, x_\beta} \psi_\alpha(x_\alpha) \psi_\beta(x_\beta) \cdot s_{\alpha \setminus i}^{x_{\alpha \setminus i}} \cdot (s_k s_i)^{x_i} \cdot s_{\beta \setminus j}^{x_{\beta \setminus j}} \cdot (s_k s_j)^{x_j} \\ &= \left(\sum_{x_\alpha} \psi_\alpha(x_\alpha) \cdot s_{\alpha \setminus i}^{x_{\alpha \setminus i}} \cdot (s_k s_i)^{x_i} \right) \cdot \left(\sum_{x_\beta} \psi_\beta(x_\beta) \cdot s_{\beta \setminus j}^{x_{\beta \setminus j}} \cdot (s_k s_j)^{x_j} \right) \\ &= F_\alpha(s_{\alpha \setminus i}, s_k s_i) \cdot F_\beta(s_{\beta \setminus j}, s_k s_j) \end{aligned}$$

\square

Proof of Proposition 5. We can combine Propositions 3 and 2 to first expand the factor with a thinned variable $x_j = \rho \circ x_i$ and then observe $x_j = a$. We get

$$\begin{aligned} F'_\alpha(s_\alpha) &= \frac{1}{a!} \frac{\partial^a}{\partial s_j^a} F_\alpha(s_{\alpha \setminus i}, s_i(\rho s_j + 1 - \rho)) \Big|_{s_j=0} \\ &= \frac{1}{a!} \left(\frac{\partial^a}{\partial t_i^a} F_\alpha(s_{\alpha \setminus i}, t_i) (s_i \rho)^a \Big|_{t_i=s_i(\rho s_j + 1 - \rho)} \right) \Big|_{s_j=0} \\ &= \frac{1}{a!} (s_i \rho)^a \frac{\partial^a}{\partial t_i^a} F_\alpha(s_{\alpha \setminus i}, t_i) \Big|_{t_i=s_i(1-\rho)}. \end{aligned}$$

\square

Algorithm 4 PGF-FORWARD implementation

Input: Vectors λ, δ, ρ, y
Output: Likelihood $p(y_{1:K})$

```
1:  $a \leftarrow 0, b \leftarrow 0, f(s) \leftarrow 1$ 
2: for  $k = 1$  to  $K$  do
3:    $[a, b] \leftarrow \text{ARRIVALS}(a, b, \lambda_k)$ 
4:    $[a, f] \leftarrow \text{EVIDENCE}(a, f, y_k, \rho_k)$ 
5:   if  $k < K$  then
6:      $[a, b, f] \leftarrow \text{SURVIVORS}(a, b, f, \delta_k)$ 
7:   end if
8: end for
9: return  $f(1) \exp\{a + b\}$ 

10: function  $\text{ARRIVALS}(a, b, \lambda)$ 
11:    $a' \leftarrow a + \lambda$ 
12:    $b' \leftarrow b - \lambda$ 
13:   return  $a', b'$ 
14: end function

15: function  $\text{EVIDENCE}(a, f, y, \rho)$ 
16:    $a' \leftarrow a(1 - \rho)$ 
17:    $g \leftarrow 0, df \leftarrow f$ 
18:   for  $\ell = 0$  to  $y$  do
19:      $g \leftarrow g + df / (a^\ell \ell! (y - \ell)!)$ 
20:      $df \leftarrow \text{DERIV}(df)$ 
21:   end for
22:    $g \leftarrow \text{COMPOSE}(g, s(1 - \rho))$ 
23:    $g \leftarrow (a\rho)^y s^y g$ 
24:   return  $a', g$ 
25: end function

26: function  $\text{SURVIVORS}(a, b, f, \delta)$ 
27:    $a' \leftarrow a\delta$ 
28:    $b' \leftarrow b + a(1 - \delta)$ 
29:    $f' \leftarrow \text{COMPOSE}(f, \delta s + 1 - \delta)$ 
30:   return  $a', b', f'$ 
31: end function
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Proof of Proposition 6. This is an immediate consequence of Proposition 3 and Proposition 1 by setting $s_i = 1$ in Proposition 3. \square

Proof of Proposition 7. This is an immediate consequence of Proposition 4 and Proposition 1 by setting $s_i = 1$ and $s_j = 1$ in Proposition 4. \square

B Implementation of PGF-FORWARD

The detailed algorithm, based on the proof of Theorem 1, is listed in Algorithm 4.

Here is the proof of the runtime result (Theorem 2):

Proof of Theorem 2. We assume a polynomial f is represented as a vector of coefficients $\{f_i\}$ of length $\deg(f) + 1$. ARRIVALS takes constant time. The running time of EVIDENCE is $\mathcal{O}(y \deg(f)) = \mathcal{O}(Y^2)$: Lines 19 and 20 are executed y times and take time proportional to $\deg(g)$ and $\deg(df)$, respectively, each of which is no more than $\deg(f)$. The operations outside the loop are bounded by $\mathcal{O}(y + \deg(f))$. (Note that the COMPOSE operation in Line 22 is linear in $\deg(g)$ —simply multiply the i th coefficient of g by $(1 - \rho)^i$ for all i .) The SURVIVORS function takes $\mathcal{O}(Y^2)$ time. The COMPOSE operation in Line 29 is more costly than the one on Line 22: we must expand $\sum_i g_i (\delta s + 1 - \delta)^i$ to compute the coefficients of s^i for all i —this can be done in $\mathcal{O}(\deg(g)^2)$ time by a number of methods, e.g., applying the Binomial Theorem to expand each term. The ARRIVALS, EVIDENCE, and SURVIVORS functions are each called K or $K - 1$ times. Therefore, the overall running time is $\mathcal{O}(KY^2)$. \square

C Implementation of PGF-TAIL-ELIMINATE

We provide a side-by-side comparison of PGF-TAIL-ELIMINATE with a non-PGF implementation of the equivalent algorithm, TAIL-ELIMINATE, in Figure 7. The detailed PGF-TAIL-ELIMINATE algorithm is listed in Algorithm 7.

Proof of Theorem 3. We again proceed inductively. From the proof of Theorem 1, we initially have that $A_i(s) = f(s) \exp\{as + b\}$ where $\deg(f) = \sum_{k=1}^i y_k$. Then, in Line 1, we have

$$\Psi_{i,i+1}(s, t) = f(s(\delta_i t + 1 - \delta_i)) \exp\{a\delta_i s t + a(1 - \delta_i)s + b\}$$

The first term is a bivariate polynomial $f'(s, t) := \sum_{i=0}^{\deg(f)} f_i s^i (\delta_i t + 1 - \delta_i)^i$ with max-degree equal to $\deg(f)$, and the second term has the desired exponential form.

Algorithm 5 TAIL-ELIMINATE

Output: Unnormalized marginal $p(n_i, y_{1:K})$

- 1: $\phi_{i,i+1}(n_i, z_{i+1}) := \alpha_i(n_i)p(z_{i+1}|n_i)$
- 2: **for** $j = i + 1$ to K **do**
- 3: $\eta_{ij}(n_i, n_j) := \sum_{m_j, z_j} \phi(n_i, z_j)p(m_j)p(n_j|z_j, m_j)$
- 4: $\theta_{ij}(n_i, n_j) := \eta_{ij}(n_i, n_j)p(y_j|n_j)$
- 5: **if** $j < K$ **then**
- 6: $\phi_{i,j+1}(n_i, z_{j+1}) := \theta_{ij}(n_i, n_j)p(z_j|n_{j-1})$
- 7: **end if**
- 8: **end for**
- 9: **return** $p(n_i, y_{1:K}) = \sum_{n_K} \theta_{iK}(n_i, n_K)$

Algorithm 6 PGF-TAIL-ELIMINATE

Output: PGF of unnormalized marginal $p(n_i, y_{1:K})$

- 1: $\Phi_{i,i+1}(s, t) := A_i(s(\delta_i t + 1 - \delta_i))$
- 2: **for** $j = i + 1$ to K **do**
- 3: $H_{ij}(s, t) := \Phi_{ij}(s, t) \exp\{\lambda_k(t - 1)\}$
- 4: $\Theta_{ij}(s, t) := \frac{1}{y_j!} (t\rho_j)^{y_j} \frac{\partial^{y_j} H_{ij}(s, u)}{\partial u^{y_j}} \Big|_{u=t(1-\rho_j)}$
- 5: **if** $j < K$ **then**
- 6: $\Phi_{i,j+1}(s, t) := \Theta_{ij}(s, \delta_j t + 1 - \delta_j)$
- 7: **end if**
- 8: **end for**
- 9: **return** $\Theta_{iK}(s, 1)$

Figure 7: Comparison of the PGF-TAIL-ELIMINATE algorithm with its equivalent using non-PGF factors, TAIL-ELIMINATE.

In Line 3, suppose $\Phi_{ij}(s, t) = f(s, t) \exp\{ast + bs + ct + d\}$. Then $H_{ij}(s, t) = f(s, t) \exp\{ast + cs + (c + \lambda_k)t + (d - \lambda_k)\}$, which has the desired form.

In Line 4, the suppose $H_{ij}(s, u) = f(s, u) \exp\{ast + bs + cu + d\}$. One can verify by calculating the y th partial derivative of H_{ij} with respect to u that:

$$\Theta_{ij}(s, t) = \rho_j^{y_j} \cdot \left(t^{y_j} \sum_{\ell=0}^{y_j} \frac{(as + c)^{y_j - \ell}}{\ell!(y_j - \ell)!} \cdot \frac{\partial^\ell f(s, u)}{\partial u^\ell} \Big|_{u=t(1-\rho_j)} \right) \cdot \exp\{a(1-\rho_j)st + bs + c(1-\rho)t + d\}$$

The term in parentheses is again a bivariate polynomial—the largest exponent of s and t have both increased by y_j , so the max-degree increases by y_j . The exponential term is in the desired form and can absorb the scalar ρ^{y_j} . Therefore, in Line 4, $\Theta_{ij}(s, t)$ has the desired form, and the degree of the polynomial part of the representation increases by y_j .

In Line 6, suppose $\Theta_{ij}(s, t) = f(s, t) \exp\{ast + bs + ct + d\}$. Then $\Phi_{i,j+1}(s, t) = g(s, t) \exp\{a\delta_k st + (b + a(1 - \delta_k))s + c\delta_k t + (d + c(1 - \delta_k))\}$, where $g(s, t) = f(s, h(t))$ is the composition of f with the affine function $h(t) = \delta_k t + 1 - \delta_k$, so g is a bivariate polynomial of the same degree as f . Therefore, $\Phi_{i,j+1}(s, t)$ has the desired form.

We have shown that each PGF retains the desired form. Furthermore, the max-degree of the polynomial is initially equal to $\sum_{k=1}^i y_k$ and increases by y_j for all $j = i + 1$ to K , so it is always bounded by $Y = \sum_{k=1}^K y_k$. \square

Proof of Theorem 4 (PGF-TAIL-ELIMINATE running time). We assume for simplicity that all polynomials have max-degree equal to the upper bound Y . A bivariate polynomial is represented as a matrix of Y^2 coefficients for the monomials $s^i t^j$.

The running time of INIT-SURVIVORS function is dominated by Line 16, which takes $\mathcal{O}(Y^2)$ time. For each term in the sum, the coefficients of the polynomial $(\delta t + 1 - \delta)^i$ can be computed in $\mathcal{O}(i) = \mathcal{O}(Y)$ time (e.g., by the Binomial Theorem) and then multiplied by f_i to determine the coefficients of $s^i t^j$ for all j . This repeats $\mathcal{O}(Y)$ times, once for each term in the sum.

The running time of ARRIVALS is $\mathcal{O}(1)$.

The running time of SURVIVORS is $\mathcal{O}(Y^3)$. The COMPOSE operation in Line 41 can be structured as

$$\sum_{i,j} f_{ij} s^i (\delta t + 1 - \delta)^j = \sum_i s^i \sum_j f_{ij} (\delta t + 1 - \delta)^j$$

For each value of i , we compose the univariate polynomial $\sum_j f_{ij} t^j$ with the affine function $\delta t + 1 - \delta$. This can be done in $\mathcal{O}(Y^2)$ time, as in the proof of Theorem 2, for a total running time of $\mathcal{O}(Y^3)$. \square

Algorithm 7 PGF-TAIL-ELIMINATE implementation

Input: Vectors λ, δ, ρ, y , index i , parameters f, a, b of initial PGF $A_i(s) = f(s) \exp\{as + b\}$ (from PGF-FORWARD)

Output: Final PGF for unnormalized marginal $p(n_i, y_{1:K})$ in form $f(s) \exp\{as + b\}$

```
1: // Initialize:  $f(s, t) \exp\{ast + bs + ct + d\}$ 
2:  $[a, b, c, d, f] \leftarrow \text{INIT-SURVIVORS}(a, b, f, \delta_i)$ 
3: for  $j = i + 1$  to  $K$  do
4:    $[c, d] \leftarrow \text{ARRIVALS}(c, d, \lambda_k)$ 
5:    $[a, c, f] \leftarrow \text{EVIDENCE}(a, c, f, y_k, \rho_k)$ 
6:   if  $k < K$  then
7:      $[a, b, c, d, f] \leftarrow \text{SURVIVORS}(a, b, c, d, f, \delta_k)$ 
8:   end if
9: end for
10: return  $f(s, 1) \exp\{(a + b)s + (c + d)\}$ 

11: function INIT-SURVIVORS( $a, b, f, \delta$ )
12:    $a' \leftarrow a\delta$ 
13:    $b' \leftarrow b(1 - \delta)$ 
14:    $c' \leftarrow 0$ 
15:    $d' \leftarrow b$ 
16:    $f'(s, t) \leftarrow \sum_i f_i s^i (\delta t + 1 - \delta)^i$ 
17:   return  $a', b', c', d', f'$ 
18: end function

19: function ARRIVALS( $c, d, \lambda$ )
20:    $c' \leftarrow c + \lambda$ 
21:    $d' \leftarrow d - \lambda$ 
22:   return  $c', d'$ 
23: end function

24: function EVIDENCE( $a, c, f, y, \rho$ )
25:    $a' \leftarrow a(1 - \rho)$ 
26:    $c' \leftarrow c(1 - \rho)$ 
27:    $g \leftarrow 0, df \leftarrow f$ 
28:   for  $\ell = 0$  to  $y$  do
29:      $g \leftarrow g + \frac{\text{MULT}(df, (as + c)^{y-\ell})}{\ell!(y - \ell)!}$ 
30:      $df \leftarrow \text{PARTIAL}(df, t)$ 
31:   end for
32:    $g \leftarrow \text{COMPOSE}(g, t(1 - \rho))$ 
33:    $g \leftarrow \rho^y s^y g$ 
34:   return  $a', g$ 
35: end function

36: function SURVIVORS( $a, b, f, \delta$ )
37:    $a' \leftarrow a\delta$ 
38:    $b' \leftarrow b + a(1 - \delta)$ 
39:    $c' \leftarrow c\delta$ 
40:    $d' \leftarrow d + c(1 - \delta)$ 
41:    $f' \leftarrow \text{COMPOSE}(f, \delta t + 1 - \delta)$ 
42:   return  $a', b', f'$ 
43: end function
```

The total running time of PGF-TAIL-ELIMINATE *excluding* the EVIDENCE function is therefore $\mathcal{O}(KY^3)$.

The running time of one call to EVIDENCE is $\mathcal{O}(yY^2 \log Y)$. It is dominated by Line 29. The multiplication in this line can be structured as

$$\left(\sum_{i,j} (df)_{ij} s^i t^j \right) (as + c)^{y-\ell} = \sum_j t^j \left(\sum_i (df)_{ij} s^i \right) (as + c)^{y-\ell}$$

For each value of j , we multiply two univariate polynomials in s whose total degree is at most Y . This can be done in time $\mathcal{O}(Y \log Y)$ using a fast Fourier transform. We repeat this at most $Y \cdot y$ times—once for each possible value of j and ℓ . The total running time of a single call to EVIDENCE is therefore $\mathcal{O}(yY^2 \log Y)$. The total running time of all calls to the evidence function is $\mathcal{O}(\sum_{j=i+1}^K y_k Y^2 \log Y) = \mathcal{O}(Y^3 \log Y)$.

The overall running time is therefore $\mathcal{O}(Y^3(K + \log Y))$.

D Proof of Theorem 5 — Extracting Marginal Probabilities and Moments

Proof of Theorem 5. We assume for the proof that the PGF is already normalized, which can be done by setting $b \leftarrow b - \log Z$. For (i) and (ii), we use the following standard facts about PGFs:

$\mu = F^{(1)}(1)$ and $\sigma^2 = F^{(2)}(1) - \mu^2 + \mu$ [3]. Then we have:

$$\begin{aligned}\mu &= F^{(1)}(1) = \left. \frac{d}{ds} f(s)e^{as+b} \right|_{s=1} \\ &= f'(1)e^{a+b} + af(1)e^{a+b} \\ &= e^{a+b} \sum_{i=0}^m (mf_i + af_i) \\ &= e^{a+b} \sum_{i=0}^m (a+m)f_i\end{aligned}$$

And

$$\begin{aligned}F^{(2)}(1) &= \left. \frac{d^2}{ds^2} f(s)e^{as+b} \right|_{s=1} \\ &= f^{(2)}(1)e^{a+b} + 2f^{(1)}(1)ae^{a+b} + a^2f(1) \\ &= e^{a+b} \left(f^{(2)}(1) + 2af^{(1)}(1) + a^2f(1) \right) \\ &= e^{a+b} \sum_{i=0}^m (m(m-1)f_i + 2amf_i + a^2f_i) \\ &= e^{a+b} \sum_{i=0}^m ((a+m)^2 - m)f_i\end{aligned}$$

For part (iii), we use the following standard fact about the Taylor expansion of the exponential:

$$e^{as} = \sum_{j=0}^{\infty} \frac{a^j}{j!} s^j$$

Then we have:

$$\begin{aligned}F(s) &= \left(\sum_{i=0}^m f_i s^i \right) e^{as+b} \\ &= e^b \left(\sum_{i=0}^m f_i s^i \right) \left(\sum_{j=0}^{\infty} \frac{a^j}{j!} s^j \right) \\ &= e^b \sum_{i=0}^m \sum_{j=0}^{\infty} f_i \frac{a^j}{j!} s^{i+j} \\ &= e^b \sum_{\ell=0}^{\infty} s^{\ell} \sum_{i=0}^{\min\{m,\ell\}} f_i \frac{a^{\ell-i}}{(\ell-i)!}\end{aligned}$$

The final expression reveals the unique explicit representation of the PGF as a formal power series in s . The coefficient of s^{ℓ} , which is equal to the value of the PMF at ℓ , is $e^b \sum_{i=0}^{\min\{m,\ell\}} f_i \frac{a^{\ell-i}}{(\ell-i)!}$.

□