

# Counting distributions in Bayesian networks and Markov models with polynomials

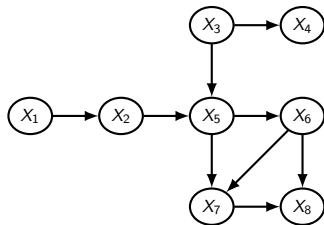
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# Bayesian networks - DAG - and belief propagation



$$\mathcal{X}_{\mathcal{U}} = \{X_u\}_{u \in \mathcal{U}}$$
$$\forall u \in \mathcal{U}, X_u \in \mathcal{X}_u$$

$\text{pa}_u$  : set of labels for parents of  $X_u$

$$\sum_{\mathcal{X}_{\mathcal{U}}} \prod_{u \in \mathcal{U}} \mathbb{P}(X_u | X_{\text{pa}_u}) = 1$$

Let  $\overline{X}_u = \{X_u, X_{\text{pa}_u}\}$ ,

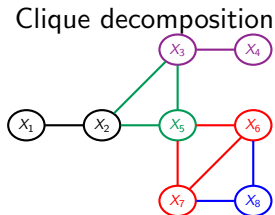
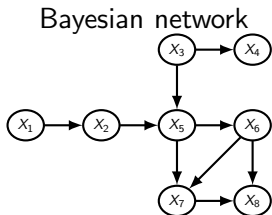
$$\text{ev} = \{X_u \in \mathcal{X}_u^* \subset \mathcal{X}_u\} \rightarrow \varphi_{X_u}(\overline{X}_u) = \mathbb{1}_{X_u \in \mathcal{X}_u^*} \mathbb{P}(X_u | X_{\text{pa}_u})$$

$$\mathbb{P}(\text{ev}) = \sum_{\mathcal{X}_{\mathcal{U}}} \prod_{u \in \mathcal{U}} \varphi_{X_u}(\overline{X}_u)$$

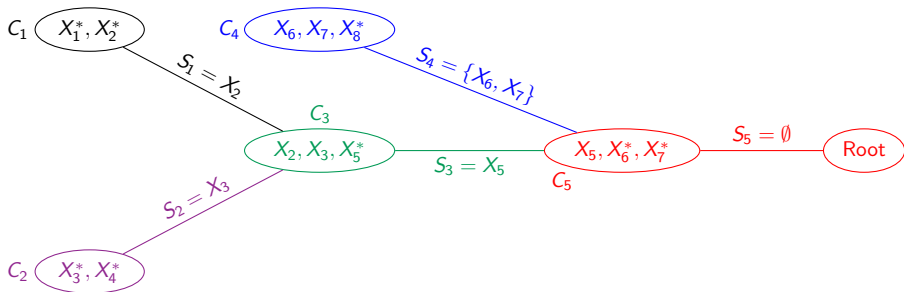
$$\forall v \in \mathcal{U}, \mathbb{P}(X_v, \text{ev}) = \sum_{\mathcal{X}_{\mathcal{U} \setminus X_v}} \prod_{u \in \mathcal{U}} \varphi_{X_u}(\overline{X}_u)$$

Complexity =  $\mathcal{O}(\prod_u |\mathcal{X}_u|)$ , ie  $\mathcal{O}(2^n)$  for only binary variables.

# Message passing or sum-product algorithm



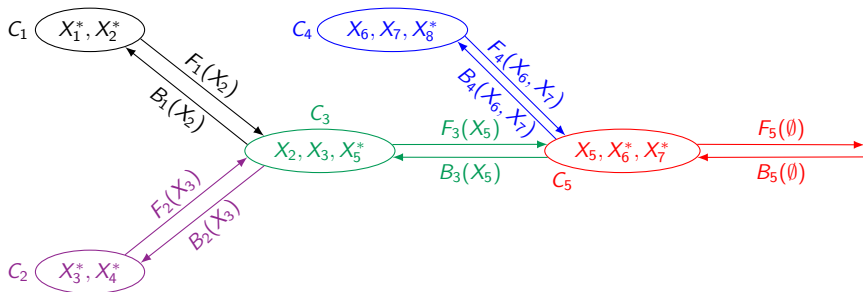
$$\begin{aligned}
 \mathbb{P}(\text{ev}) = & \sum_{X_5} \sum_{X_6} \sum_{X_7} \left\{ \sum_{X_8} \varphi_{X_8}(\bar{X}_8) \right. \\
 & \sum_{X_2} \sum_{X_3} \left( \underbrace{\sum_{X_1} \varphi_{X_1}(\bar{X}_1) \varphi_{X_2}(\bar{X}_2)}_{F_1(X_2)} \underbrace{\sum_{X_4} \varphi_{X_3}(\bar{X}_3) \varphi_{X_4}(\bar{X}_4) \varphi_{X_5}(\bar{X}_5)}_{F_2(X_3)} \right) \\
 & \left. \varphi_{X_6}(\bar{X}_6) \varphi_{X_7}(\bar{X}_7) \right\}
 \end{aligned}$$



- Junction-tree properties :

- Tree
- Running intersection
- Covering

# Message passing



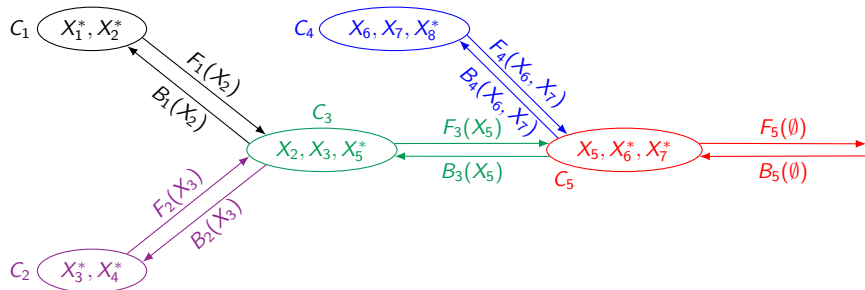
$$\forall i \in \{1, \dots, K\}; \quad \phi_i(C_i) = \prod_{X_u \in C_i} \varphi_{X_u}(\overline{X_u})$$

$$F_i(S_i) = \sum_{C_i \setminus S_i} \left( \prod_{j \in \text{from}_i} F_j(S_j) \right) \times \phi_i(C_i)$$

$$B_K(\emptyset) = 1 \text{ and for } k \in K, \dots, 1, \forall i \in \text{from}_k,$$

$$B_i(S_i) = \sum_{C_k \setminus S_i} \phi_k(S_k) \times B_k(S_k) \times \prod_{j \in \text{from}_k, j \neq i} F_j(S_j)$$

# Message passing



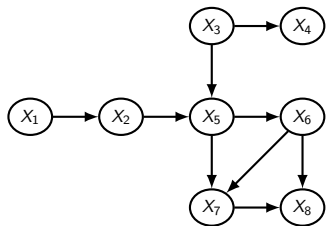
$\forall i \in \{1, \dots, K\},$

$$\mathbb{P}(S_i, \text{ev}) = F_i(S_i) \times B_i(S_i)$$

$$\mathbb{P}(C_i, \text{ev}) = \phi_i(C_i) \times B_i(S_i) \times \prod_{j \in \text{from}_i, j \neq i} F_j(S_j)$$

Complexity =  $\mathcal{O}(n \times \arg\max_u |\mathcal{X}_u|^{\text{TW}})$ , TW = size of the largest clique

Idea : Change definition of  $ev$  and work on the arithmetic of potentials to compute other quantities of interest.



$$\mathcal{X}_{\mathcal{U}} = \{X_u\}_{u \in \mathcal{U}}$$

$$\forall u \in \mathcal{U}, X_u \in \mathcal{X}_u$$

$\text{pa}_u$  : set of labels for parents of  $X_u$

$$\sum_{\mathcal{X}_{\mathcal{U}}} \prod_{u \in \mathcal{U}} \mathbb{P}(X_u | \mathcal{X}_{\text{pa}_u}) = 1$$

Let  $\overline{\mathcal{X}}_u = \{X_u, \mathcal{X}_{\text{pa}_u}\}$

$$ev = \{X_u \in \mathcal{X}_u^* \subset \mathcal{X}_u\} \rightarrow \varphi_{X_u}(\overline{\mathcal{X}}_u) = \mathbb{1}_{X_u \in \mathcal{X}_u^*} \mathbb{P}(X_u | \mathcal{X}_{\text{pa}_u})$$

$$\mathbb{P}(ev) = \sum_{\mathcal{X}_{\mathcal{U}}} \prod_{u \in \mathcal{U}} \varphi_{X_u}(\overline{\mathcal{X}}_u)$$

$$\forall v \in \mathcal{U}, \mathbb{P}(X_v, ev) = \sum_{\mathcal{X}_{\mathcal{U} \setminus X_v}} \prod_{u \in \mathcal{U}} \varphi_{X_u}(\overline{\mathcal{X}}_u)$$

# Derivatives of the likelihood with derivative generating functions in parametric bayesian networks.

$$\varphi_u(\overline{X}_u) = \mathbb{1}_{X_u \in \mathcal{X}_u^*} \mathbb{P}(X_u | X_{\text{pa}_u}, \theta) \quad \Rightarrow \quad \sum_{X_u} \prod_{u \in \mathcal{U}} \varphi_u(\overline{X}_u) = \mathbb{P}(\text{ev} | \theta) = L(\theta)$$

**Message passing algo.:**  $\forall i \in 1, \dots, K, \quad \sum_{S_i} F_i(S_i) B_i(S_i) = L(\theta)$

with  $K$ : Number of cliques of the built JT.

**Polynomial potentials:**  $\Phi_u(\overline{X}_u) = \sum_{k=0}^d \varphi_u^{(d)}(\overline{X}_u) z^k$

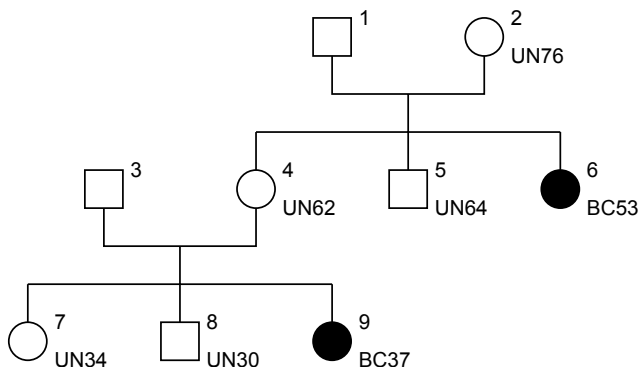
**Leibniz's product:**  $\sum_{k=0}^d a_k z^k \star \sum_{k=0}^d b_k z^k = \sum_{k=0}^d \sum_{i=0}^k \binom{i}{k} a_i b_{k-i} z^k$

**Message passing algo over polynomial potentials:**

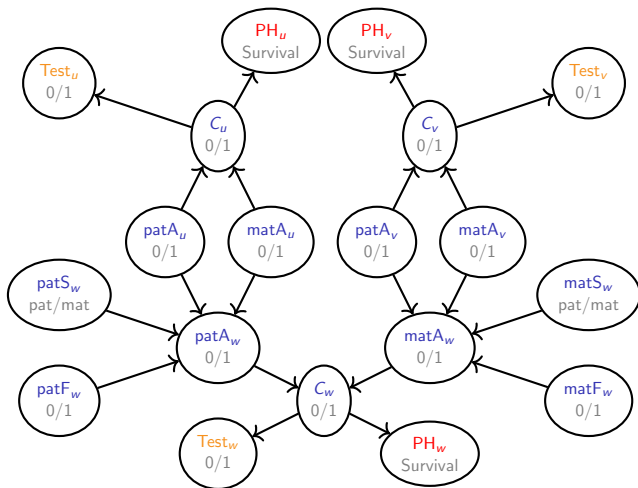
$$\forall i \in 1, \dots, K, \quad \sum_{S_i} \mathbf{F}_i(S_i) \mathbf{B}_i(S_i) = \sum_{k=0}^d L^{(k)}(\theta) z^k$$



# Counting distribution with probability and moment generating functions (Application with genetic diseases).



- Distribution of the # of carriers ( $N^C$ )
- Distribution of the # of filiation errors ( $N^F$ ) (+joint distributions)
- Moments



$$ev = \{PH_u\}_{u=1, \dots, n_{\text{ind}}} \cap \{\text{Test}_u\}_{u \in \{1, \dots, n_{\text{ind}}\}}, \quad n_{\text{ind}} = \# \text{ of ind.}$$

Probability generating function of  $N$  :  $G_N(z) = \mathbb{E}(z^N)$   
 with  $N = \sum_u C_u$  (Number of carriers).

**Evidence:**  $ev = \{\text{PH}_u\}_{u=1,\dots,n_{\text{ind}}} \cap \{\text{Test}_u\}_{u \in \{1,\dots,n_{\text{ind}}\}}$

**Polynomial Potentials:**  $\varphi_{C_u}(\overline{C}_u) = \mathbb{P}(C_u | \text{pat}A_u, \text{mat}A_u)$   
 $\Rightarrow \Phi_{C_u}(\overline{C}_u) = \mathbb{P}(C_u | \text{pat}A_u, \text{mat}A_u) z^{C_u}$

For each other variable,  $\varphi_{\cdot}(\cdot) = \Phi_{\cdot}(\cdot)$

**Computation with the Sum-product / message passing algorithm:**

With variables renamed  $X_u$ ,  $u \in \mathcal{U} = \{1, \dots, n\}$  ( $n = \#$  of variables):

$\forall i \in 1, \dots, K$  ( $K$ :  $\#$  of cliques of the built JT),

$$\begin{aligned} \sum_s \underbrace{\mathbf{F}_i(s) \times \mathbf{B}_i(s)}_{\text{Polynomial messages}} &= \sum_{X_{\mathcal{U}}} \prod_u \Phi_{X_u}(\overline{X}_u) \\ &= \sum_{k \geq 0} \mathbb{P}(N = k, ev) z^k \end{aligned}$$

# multivariate polynomials for joint distributions

$$N^C = \sum_u C_u \text{ and } N^F = \sum_u \text{pat}F_u$$

## Joint distribution of # of carriers and # of paternal filiation errors

For all individuals:  $\varphi_{C_u}(\overline{C_u}) \Rightarrow \Phi_{C_u}(\overline{C_u}) = \mathbb{P}(C_u | \text{pat}A_u, \text{mat}A_u) z^{C_u}$

For offsprings:  $\varphi_{\text{pat}F_u}(\overline{\text{pat}F_u}) \Rightarrow \Phi_{\text{pat}F_u}(\overline{\text{pat}F_u}) = \mathbb{P}(\text{pat}F_u) y^{\text{pat}F_u}$

## Computation with the sum-product / message-passing algorithm:

With variables renamed  $X_u$ ,  $u \in \mathcal{U} = \{1, \dots, n\}$  ( $n = \#$  of variables):

$\forall i \in 1, \dots, K$  ( $K$ : # of cliques of the built JT),

$$\begin{aligned} \sum_s \underbrace{\mathbf{F}_i(s) \times \mathbf{B}_i(s)}_{\text{Polynomial messages}} &= \sum_{X_{\mathcal{U}}} \prod_u \Phi_{X_u}(\overline{X_u}) \\ &= \sum_{k \geq 0} \sum_{\ell \geq 0} \mathbb{P}(N^C = k, N^F = \ell, \text{ev}) z^k y^\ell \end{aligned}$$

# Moment generating function of $N$ : $M_N(t) = \mathbb{E}(e^{tN})$

**Polynomial potentials:**  $\varphi_{C_u}(\overline{C}_u) = \mathbb{P}(C_u | \text{pat}A_u, \text{mat}A_u)$

$$\Rightarrow \Phi_{C_u}(\overline{C}_u) = \mathbb{P}(C_u | \text{pat}A_u, \text{mat}A_u) e^{tC_u}$$

$$\Rightarrow \Phi_{C_u}(\overline{C}_u) = \mathbb{P}(C_u | \text{pat}A_u, \text{mat}A_u) \left[ \sum_{\ell=0}^d \frac{t^\ell}{\ell!} \right]^{C_u} \text{ with } d, \text{ a chosen order.}$$

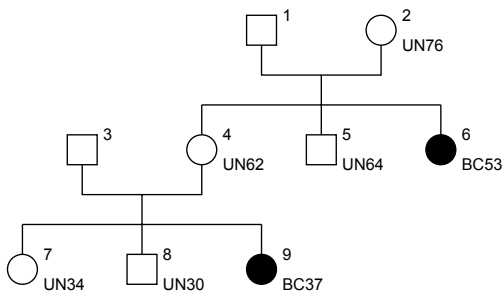
For each other variable,  $\varphi(\cdot) = \Phi(\cdot)$

**Computation with the sum-product / message-passing algorithm:**

$\forall i \in 1, \dots, K,$

$$\begin{aligned} \sum_s \underbrace{\mathbf{F}_i(s) \times \mathbf{B}_i(s)}_{\text{Polynomial messages}} &= \sum_{m \geq 0} \mathbb{P}(N = m, \text{ev}) e^{mt} \\ &= \sum_{m \geq 0} \sum_{\ell=0}^d \mathbb{P}(N = m, \text{ev}) \frac{m^\ell t^\ell}{\ell!} = \sum_{\ell=0}^d \underbrace{\left\{ \sum_{m \geq 0} \mathbb{P}(N = m, \text{ev}) m^\ell \right\}}_{\mathbb{E}[N^\ell, \text{ev}]} \frac{t^\ell}{\ell!} \end{aligned}$$

# Results



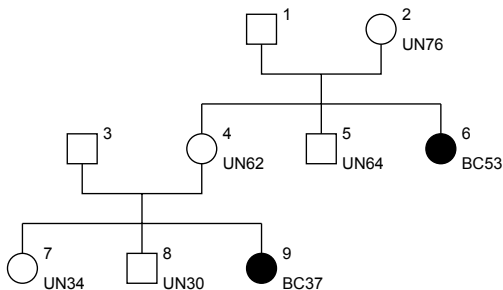
$$\pi(\cdot) = \mathbb{P}(\cdot | \text{FH})$$

2/3	2/4	2/6	2/9	$\pi(C_{\mathcal{J}})$
0	0	0	0	67.5
0	1	1	1	18.0
1	0	0	1	10.0
0	0	1	0	1.9
0	1	0	1	1.4
0	1	1	0	0.4

Individual $i$	$\pi(N)$	2/1	2/2	2/3	2/4	2/5	2/6	2/7	2/8	2/9
$\pi(C_i = 1)$	—	17.3	5.1	10.7	20.0	11.1	20.8	14.7	15.2	30.0
$\pi(C_i = 1   N = 0)$	67.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
$\pi(C_i = 1   N = 5)$	7.6	<b>77.6</b>	22.4	1.6	<b>98.5</b>	36.9	<b>93.1</b>	34.7	37.0	<b>98.1</b>
$\pi(C_i = 1   N = 6)$	7.0	<b>77.6</b>	22.6	2.1	<b>98.5</b>	68.1	<b>97.5</b>	66.0	68.3	<b>99.3</b>
$\pi(C_i = 1   N = 3)$	6.2	14.6	4.2	<b>81.1</b>	4.1	14.8	15.6	39.7	42.5	<b>83.5</b>
$\pi(C_i = 1   N = 4)$	5.5	44.0	12.6	44.2	55.7	4.4	46.6	47.5	47.8	<b>97.1</b>
$\pi(C_i = 1   N = 2)$	3.8	20.9	5.9	73.1	0.3	1.9	24.8	1.4	1.5	70.4

3 founders, 6 offsprings, 60 variables, 41 cliques, complexity 748

# Results



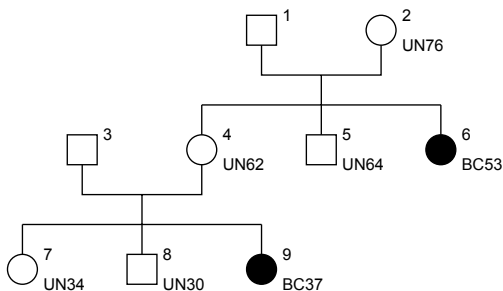
$$\pi(\cdot) = \mathbb{P}(\cdot | \text{FH}, T_4 = 1)$$

2/3	2/4	2/6	2/9	$\pi(C_{\mathcal{J}})$
0	1	1	1	81.8
0	0	0	0	7.7
0	1	0	1	6.4
0	1	1	0	1.7
1	0	0	1	1.1
1	1	1	1	0.8

Individual $i$	$\pi(N)$	2/1	2/2	2/3	2/4	2/5	2/6	2/7	2/8	2/9
$\pi(C_i = 1)$	—	70.8	20.7	2.0	<b>90.9</b>	45.4	<b>84.6</b>	44.6	46.2	<b>90.2</b>
$\pi(C_i = 1   N = 5)$	34.1	<b>77.6</b>	22.4	0.2	<b>100</b>	36.9	<b>93.1</b>	34.7	37.0	<b>98.1</b>
$\pi(C_i = 1   N = 6)$	31.3	<b>77.6</b>	22.6	0.7	<b>100</b>	68.0	<b>97.5</b>	66.0	68.3	<b>99.3</b>
$\pi(C_i = 1   N = 4)$	14.1	<b>76.2</b>	21.8	2.0	<b>98.1</b>	7.6	<b>80.5</b>	9.2	9.7	<b>95.0</b>
$\pi(C_i = 1   N = 7)$	10.2	<b>77.7</b>	23.6	3.8	<b>100</b>	<b>97.4</b>	<b>99.8</b>	<b>98.9</b>	<b>99.0</b>	<b>100</b>
$\pi(C_i = 1   N = 0)$	7.6	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
$\pi(C_i = 1   N = 3)$	1.8	51.5	14.6	31.2	63.1	6.6	18.0	17.4	18.7	<b>78.9</b>

3 founders, 6 offsprings, 60 variables, 41 cliques, complexity 748

# Results



$$\pi(\cdot) = \mathbb{P}(\cdot | \text{FH}, T_4 = 0)$$

2/3	2/4	2/6	2/9	$\pi(C_{\mathcal{J}})$
0	0	0	0	80.3
1	0	0	1	11.9
0	1	1	1	4.4
0	0	1	0	2.2
0	1	0	1	0.3
1	0	1	1	0.3

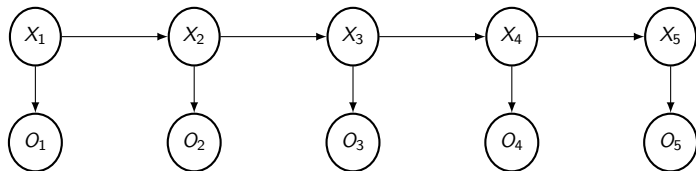
Individual $i$	$\pi(N)$	2/1	2/2	2/3	2/4	2/5	2/6	2/7	2/8	2/9
$\pi(C_i = 1)$	—	5.9	1.7	12.5	4.9	3.8	7.1	8.3	8.6	17.1
$\pi(C_i = 1   N = 0)$	80.1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
$\pi(C_i = 1   N = 3)$	7.1	12.6	3.6	<b>83.9</b>	0.9	15.2	15.5	40.9	43.8	<b>83.7</b>
$\pi(C_i = 1   N = 2)$	4.5	20.9	5.9	73.2	0.1	1.9	24.9	1.4	1.5	70.4
$\pi(C_i = 1   N = 4)$	3.6	17.2	4.9	<b>79.5</b>	20.4	1.8	18.2	<b>79.5</b>	<b>79.6</b>	<b>98.8</b>
$\pi(C_i = 1   N = 5)$	2.0	<b>77.6</b>	22.4	7.2	<b>93.0</b>	36.9	<b>93.1</b>	34.8	37.1	<b>98.1</b>
$\pi(C_i = 1   N = 6)$	1.8	<b>77.6</b>	22.6	7.5	<b>93.1</b>	68.1	<b>97.5</b>	66.0	68.3	<b>99.3</b>

3 founders, 6 offsprings, 60 variables, 41 cliques, complexity 748

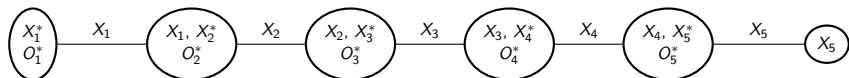


Number of errors in a Markov Chain,  $N = \sum_i \mathbb{1}_{X_i \neq 0}$

## Hidden Markov chain



## Junction tree



## Potentials

$$\varphi_{X_1}(X_1) = \mu_1; \varphi_{X_i}(\bar{X}_i) = \pi(X_{i-1}, X_i) \text{ with } \pi = \begin{pmatrix} 0.9 & 0.1 \\ 0.2 & 0.8 \end{pmatrix}$$

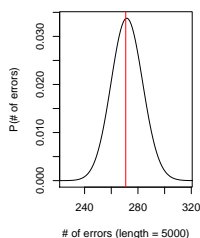
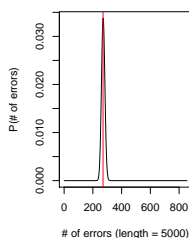
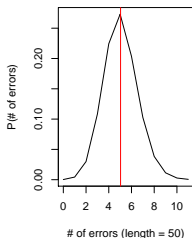
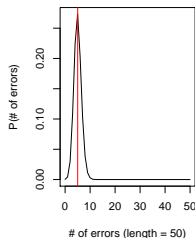
$$\text{PGF: } \varphi_{O_i}(O_i, X_i = j) = \underbrace{\mathbb{1}_{O_i = \omega_j}}_{\text{ev}} (1 - \eta)^{\mathbb{1}_{O_i = j}} (\eta \times z)^{\mathbb{1}_{O_i \neq j}} \text{ with } \eta = 0.05$$

$$\text{MGF: } \varphi_{O_i}(O_i, X_i = j) = \underbrace{\mathbb{1}_{O_i = \omega_j}}_{\text{ev}} (1 - \eta)^{\mathbb{1}_{O_i = j}} (\eta(1 + t + t^2/2 + \dots))^{\mathbb{1}_{O_i \neq j}}$$

$$\text{PGF: } \forall i \in 1, \dots, K, \quad \sum_{X_i} \mathbf{F}_i(X_i) \mathbf{B}_i(X_i) = \sum_{k \geq 0} \mathbb{P}(N = k, \text{ev}) z^k$$

$$\text{MGF: } \forall i \in 1, \dots, K, \quad \sum_{X_i} \mathbf{F}_i(X_i) \mathbf{B}_i(X_i) = \sum_{l \geq 0} \mathbb{E}[N^l, \text{ev}] \frac{t^l}{l!}$$

### Distributions:



### Moments:

$$m_0 = 1.00, \quad m_1 = 5.04, \quad m_2 = 27.63$$

$$m_0 = 1.00, \quad m_1 = 270.85, \quad m_2 = 73501.20$$

# Number of atypical segments in a sequence

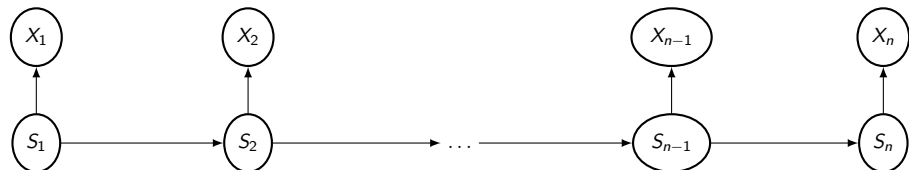
## Joint work with S. Mercier

Observed variables:  $X = X_1, \dots, X_n \in \mathcal{X}^n$  (e.g.  $\mathcal{X} = \{A, C, G, T\}$ )

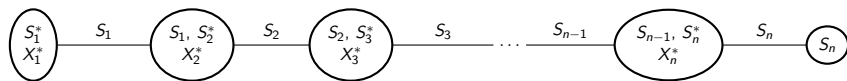
Latent variables:  $S = S_1, \dots, S_n \in \mathcal{S}^n$  ( $\mathcal{S} = \{1, 2, 3\}$ )

Emission:  $\mathbb{P}(X_i|S_i) = \begin{cases} q_0(X_i) & \text{if } S_i \neq 2 \\ q_1(X_i) & \text{if } S_i = 2 \end{cases}$     Constr. transition  $\pi = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 0 & 0 & 1 \end{pmatrix}$

### DAG



### Junction tree



- **Evidence:**  $\forall x \in \mathcal{X}, e(x) = \frac{q_1(x)}{q_0(x)}$  or  $e(x) = \exp\left(\frac{f(x)}{T}\right)$

- **Potentials:**

$$\phi_1(S_1 = k) = \pi(1, k)e(x_1)^{\mathbb{1}_{k=2}}$$

$$\text{For } i = 2, \dots, n \quad \phi_i(S_{i-1} = j, S_i = k) = \pi(j, k)e(x_i)^{\mathbb{1}_{k=2}}$$

- **Forward - Backward:**

$$F_1(S_1) = \phi_1(S_1) \quad \text{and for } i = 2, \dots, n \quad F_i(k) = \sum_j F_{i-1}(j)\phi_i(j, k)$$

$$B_n(\emptyset) = 1 \text{ (conv.)} \quad \text{and for } i = n, \dots, 2, \quad B_{i-1}(j) = \sum_k \phi(j, k)B_i(k)$$

- **Start and stop of a segment**

$$\mathbb{P}(\text{Start at pos. } i): \mathbb{P}(S_i = 2, S_{i-1} = 1, X) \propto F_{i-1}(1)\phi_i(1, 2)B_i(2)$$

$$\mathbb{P}(\text{Stop at pos. } i): \mathbb{P}(S_i = 2, S_{i+1} = 3, X) \propto F_i(2)\phi_i(2, 3)B_{i+1}(3)$$

- **Probability of the sequence**  $\forall i \in \{1, \dots, n\} \mathbb{P}(X) \propto \sum_k F_i(k)B_i(k)$

## First approach

$\mathcal{S} = \{1, 2, 3, 4, 5, \dots, 2N, 2N + 1\}$  and  $\pi$  of dimension  $(2N + 1) \times (2N + 1)$

With polynomials, pgf & mgf:  $\mathcal{S} = \{0, 1\}$  and  $\pi = \begin{pmatrix} 1 & z \\ 1 & 1 \end{pmatrix}$

$$\phi_1(S_1) = e(x_1)^{\mathbb{1}_{S_1}} \pi(S_0, S_1) \quad \text{with } S_0 = 0 \text{ (conv.)}$$

$$\forall i = 2, \dots, n \quad \phi_i(j, k) = e(x_i)^{\mathbb{1}_{S_i}} \pi(j, k)$$

Forward-Backward algo  $\rightarrow$

$$\forall i \in \{1, \dots, n\} \quad F_i(S_i) B_i(S_i) \propto \sum_k \mathbb{Q}(S_i, N = k, X) z^k$$

and  $\mathbb{P}(S_i, N = k, X) \propto \mathbb{Q}(S_i, N = k, X) / \binom{n+1}{2k}$

$$\mathbb{Q}(N = k, X) \propto \left[ \sum_j F_i(j) B_i(j) \right]_{z^k}$$

and

$$\mathbb{P}(X) \propto \sum_k \mathbb{Q}(N = k, X)$$

**$\mathbb{P}(\text{any segment starts at position } i)$**

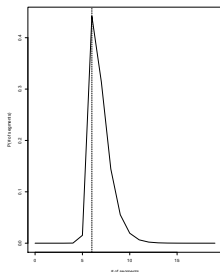
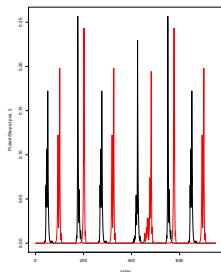
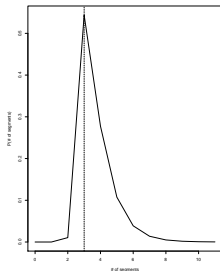
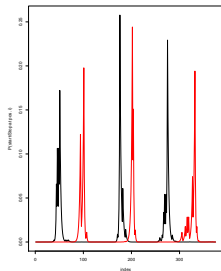
$$\mathbb{P}(S_{i-1} = 0, S_i = 1 | N = k, X) = \left[ F_{i-1}(0) B_i(1) e(X_i) \times z \right]_{z^k} / \mathbb{Q}(N = k, X)$$

**$\mathbb{P}(\text{any segment stops at position } i)$**

$$\mathbb{P}(S_i = 1, S_{i+1} = 0 | N = k, X) = \left[ F_i(1) B_{i+1}(0) \right]_{z^k} / \mathbb{Q}(N = k, X)$$

**Distribution of  $N$**

$$\mathbb{P}(N = k | X) = \frac{\mathbb{Q}(N = k, X)}{\binom{n+1}{2k} \times \mathbb{P}(X)}$$



top : simu. with 3 atypical seg. bottom: simu. with 6 atypical seg.