MCMC analysis: Outline

Transition probability $q(y \rightarrow y')$

Occupancy probability $\pi_t(y)$ at time $t$

Equilibrium condition on $\pi_t$ defines stationary distribution $\pi(y)$

Note: stationary distribution depends on choice of $q(y \rightarrow y')$

Pairwise detailed balance on states guarantees equilibrium

Gibbs sampling transition probability:

- sample each variable given current values of all others

$\Rightarrow$ detailed balance with the true posterior

For Bayesian networks, Gibbs sampling reduces to

sampling conditioned on each variable’s Markov blanket
### Stationary distribution

\[ \pi_t(y) = \text{probability in state } y \text{ at time } t \]
\[ \pi_{t+1}(y') = \text{probability in state } y' \text{ at time } t + 1 \]

\[ \pi_{t+1} \text{ in terms of } \pi_t \text{ and } q(y \to y') \]

\[ \pi_{t+1}(y') = \sum_y \pi_t(y) q(y \to y') \]

Stationary distribution: \( \pi_t = \pi_{t+1} = \pi \)

\[ \pi(y') = \sum_y \pi(y) q(y \to y') \quad \text{for all } y' \]

If \( \pi \) exists, it is unique (specific to \( q(y \to y') \))

In equilibrium, expected “outflow” = expected “inflow”
Detailed balance

“Outflow” = “inflow” for each pair of states:

\[ \pi(y)q(y \rightarrow y') = \pi(y')q(y' \rightarrow y) \quad \text{for all } y, y' \]

Detailed balance \Rightarrow \text{ stationarity:}

\[ \sum_y \pi(y)q(y \rightarrow y') = \sum_y \pi(y')q(y' \rightarrow y) \]

\[ = \pi(y')\sum_y q(y' \rightarrow y) \]

\[ = \pi(y') \]

MCMC algorithms typically constructed by designing a transition probability \( q \) that is in detailed balance with desired \( \pi \)
Gibbs sampling

Sample each variable in turn, given all other variables

Sampling $Y_i$, let $\bar{Y}_i$ be all other nonevidence variables
Current values are $y_i$ and $\bar{y}_i$; $e$ is fixed
Transition probability is given by

$$q(y \rightarrow y') = q(y_i, \bar{y}_i \rightarrow y_i', \bar{y}_i) = P(y_i' | \bar{y}_i, e)$$

This gives detailed balance with true posterior $P(y | e)$:

$$\pi(y)q(y \rightarrow y') = P(y | e)P(y_i' | \bar{y}_i, e) = P(y_i, \bar{y}_i | e)P(y_i' | \bar{y}_i, e)$$

$$= P(y_i | \bar{y}_i, e)P(\bar{y}_i | e)P(y_i' | \bar{y}_i, e) \quad \text{(chain rule)}$$

$$= P(y_i | \bar{y}_i, e)P(y_i' | \bar{y}_i | e) \quad \text{(chain rule backwards)}$$

$$= q(y' \rightarrow y)\pi(y') = \pi(y')q(y' \rightarrow y)$$