MCMC analysis: Outline

Transition probability $q(\mathbf{y} \to \mathbf{y}')$

Occupancy probability $\pi_t(\mathbf{y})$ at time t

Equilibrium condition on π_t defines stationary distribution $\pi(\mathbf{y})$
Note: stationary distribution depends on choice of $q(\mathbf{y} \to \mathbf{y}')$

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

$\pi_t(\mathbf{y})$ = probability in state $\mathbf{y}$ at time t
$\pi_{t+1}(\mathbf{y}')$ = probability in state $\mathbf{y}'$ at time $t+1$

π_{t+1} in terms of π_t and $q(\mathbf{y} \rightarrow \mathbf{y}')$

$$\pi_{t+1}(\mathbf{y}') = \Sigma_{\mathbf{y}} \pi_t(\mathbf{y}) q(\mathbf{y} \rightarrow \mathbf{y}')$$

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

$$\pi(\mathbf{y}') = \Sigma_{\mathbf{y}} \pi(\mathbf{y}) q(\mathbf{y} \rightarrow \mathbf{y}') \qquad \text{for all } \mathbf{y}'$$

If π exists, it is unique (specific to $q(\mathbf{y} \rightarrow \mathbf{y}')$)

In equilibrium, expected "outflow" = expected "inflow"

Detailed balance

"Outflow" = "inflow" for each pair of states:

$$\pi(\mathbf{y})q(\mathbf{y} \rightarrow \mathbf{y}') = \pi(\mathbf{y}')q(\mathbf{y}' \rightarrow \mathbf{y}) \qquad \text{for all } \mathbf{y},\ \mathbf{y}'$$

Detailed balance $\Rightarrow$ stationarity:

$$\begin{aligned}\Sigma_{\mathbf{y}}\pi(\mathbf{y})q(\mathbf{y} \rightarrow \mathbf{y}') &= \Sigma_{\mathbf{y}}\pi(\mathbf{y}')q(\mathbf{y}' \rightarrow \mathbf{y}) \\ &= \pi(\mathbf{y}')\Sigma_{\mathbf{y}}q(\mathbf{y}' \rightarrow \mathbf{y}) \\ &= \pi(\mathbf{y}')\end{aligned}$$

MCMC algorithms typically constructed by designing a transition probability q that is in detailed balance with desired π

Gibbs sampling

Sample each variable in turn, given *all other variables*

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

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

This gives detailed balance with true posterior $P(\mathbf{y}|\mathbf{e})$:

$$\begin{aligned}
\pi(\mathbf{y})q(\mathbf{y} \rightarrow \mathbf{y}') &= P(\mathbf{y}|\mathbf{e})P(y_i'|\bar{\mathbf{y}}_i, \mathbf{e}) = P(y_i, \bar{\mathbf{y}}_i|\mathbf{e})P(y_i'|\bar{\mathbf{y}}_i, \mathbf{e}) \\
&= P(y_i|\bar{\mathbf{y}}_i, \mathbf{e})P(\bar{\mathbf{y}}_i|\mathbf{e})P(y_i'|\bar{\mathbf{y}}_i, \mathbf{e}) \quad \text{(chain rule)} \\
&= P(y_i|\bar{\mathbf{y}}_i, \mathbf{e})P(y_i', \bar{\mathbf{y}}_i|\mathbf{e}) \qquad \text{(chain rule backwards)} \\
&= q(\mathbf{y}' \rightarrow \mathbf{y})\pi(\mathbf{y}') = \pi(\mathbf{y}')q(\mathbf{y}' \rightarrow \mathbf{y})
\end{aligned}$$