14.20 The Metropolis–Hastings algorithm is a member of the MCMC family; as such, it is designed to generate samples x (eventually) according to target probabilities π(x). (Typically we are interested in sampling from π(x)=P(x | e).) Like simulated annealing, Metropolis–Hastings operates in two stages. First, it samples a new state x′ from a proposal distribution q(x′ | x), given the current state x. Then, it probabilistically accepts or rejects x′ according to the acceptance probability:

$$\alpha(x' \mid x) = min(1,\ \frac{\pi(x') \times q(x \mid x')}{\pi(x) \times q(x' \mid x)})$$

If the proposal is rejected, the state remains at x.

a. Consider an ordinary Gibbs sampling step for a specific variable X_i. Show that this step, considered as a proposal, is guaranteed to be accepted by Metropolis–Hastings. (Hence, Gibbs sampling is a special case of Metropolis–Hastings.)
b. Show that the two-step process above, viewed as a transition probability distribution, is in detailed balance with π.

a. Consider an ordinary Gibbs sampling step for a specific variable X_i. Show that this step, considered as a proposal, is guaranteed to be accepted by Metropolis–Hastings. (Hence, Gibbs sampling is a special case of Metropolis–Hastings.)

"...the more general definition of Gibbs sampling, according to which each variable is sampled conditionally on the current values of all the other variables … satisfies the detailed balance equation with a stationary distribution equal to P(x | e), (the true posterior distribution on the nonevidence variables)." [AIMA3E, p. 538]

It is proved in the book that *"...the transition probability for each step of the Gibbs sampler is in detailed balance with the true posterior"* [AIMA3E, p. 538]

So, if the transition probability of each step is in detailed balance with the true posterior we can say that:

$$\pi(x) \times q(x \mid x_i) = \pi(x_i) \times q(x_i \mid x)\ \ for\ all\ x, x_i$$

And then the acceptance probability of the sample generated by Gibbs is:

$$\alpha(x_i \mid x) = min(1,\ \frac{\pi(x_i) \times q(x \mid x_i)}{\pi(x) \times q(x_i \mid x)}) = min(1,\ 1) = 1$$

So, the proposal is always accepted by Metropolis-Hastings.

b. Show that the two-step process above, viewed as a transition probability distribution, is in detailed balance with π.

The transition probability distribution considering the acceptance probability is:

$$q'(x \rightarrow x_i) = q'(x_i \mid x) = q(x_i \mid x) \times \alpha(x_i \mid x)$$

$$\begin{aligned}
&\pi(x) \times q'(x_i \mid x)\ = \\
&= \pi(x) \times q(x_i | x) \times \alpha(x_i | x) \\
&= \pi(x) \times q(x_i | x) \times min(1,\ \frac{\pi(x_i) \times q(x \mid x_i)}{\pi(x) \times q(x_i \mid x)})
\end{aligned}$$

$$= min(\pi(x) \times q(x_i| x),\ \frac{\pi(x) \times q(x_i| x) \times \pi(x_i) \times q(x \mid x_i)}{\pi(x) \times q(x_i \mid x)})$$
$$= min(\pi(x) \times q(x_i| x),\ \pi(x_i) \times q(x \mid x_i))$$
$$= \pi(x_i) \times q(x \mid x_i) \times min(\frac{\pi(x) \times q(x_i| x)}{\pi(x_i) \times q(x \mid x_i)},\ 1)$$
$$= \pi(x_i) \times q(x \mid x_i) \times \alpha(x \mid x_i)$$
$$= \pi(x_i) \times q'(x \mid x_i)$$

In one line:
$$\pi(x) \times q'(x_i \mid x) = \pi(x_i) \times q'(x \mid x_i)$$

Then π is in detailed balance with $q'(x_i \mid x)$

Q.E.D.