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Problem: SAMPLE FROM A DISTRIBUTION $p(x)$, without a direct sampling method.

Examples: ① SAMPLE from the posterior $p(x|y)$, where

$$p(x|y) = \frac{p(y|x)\,p(x)}{p(y)}$$

[typically $y = D$ are the data, $x = \vartheta$ are parameters of a statistical model

$$p(\vartheta|D) = \frac{p(\vartheta)\cdot p(D|\vartheta)}{p(D)}$$

PARTITION FUNCTION

$$p(y) = \underbrace{\int \underbrace{p(y|x)\,p(x)}_{p(x,y)}\,dx}$$

② MARGINALIZE from a joint distribution

$$p(x) = \int p(x,y)\,dy$$

③ EXPECTATION

$$E[f(x)] = \int f(x)\,p(x)\,dx$$

COMPUTING INTEGRALS/EXPECTATIONS

1) Sample $x_1, \dots, x_N$ from $p(x)$

2) Approximate $E[f(x)]$ with

$$I_N(f) = \frac{1}{N}\sum_{i=1}^{N} f(x_i)$$

(i.e. approx. $p(x)$ with $p_N(x) = \frac{1}{N}\sum_{i=1}^{N} \delta_{x_i}(x)$)

We know $I_N(f) \to E[f(x)]$

MCMC ALGORITHMS

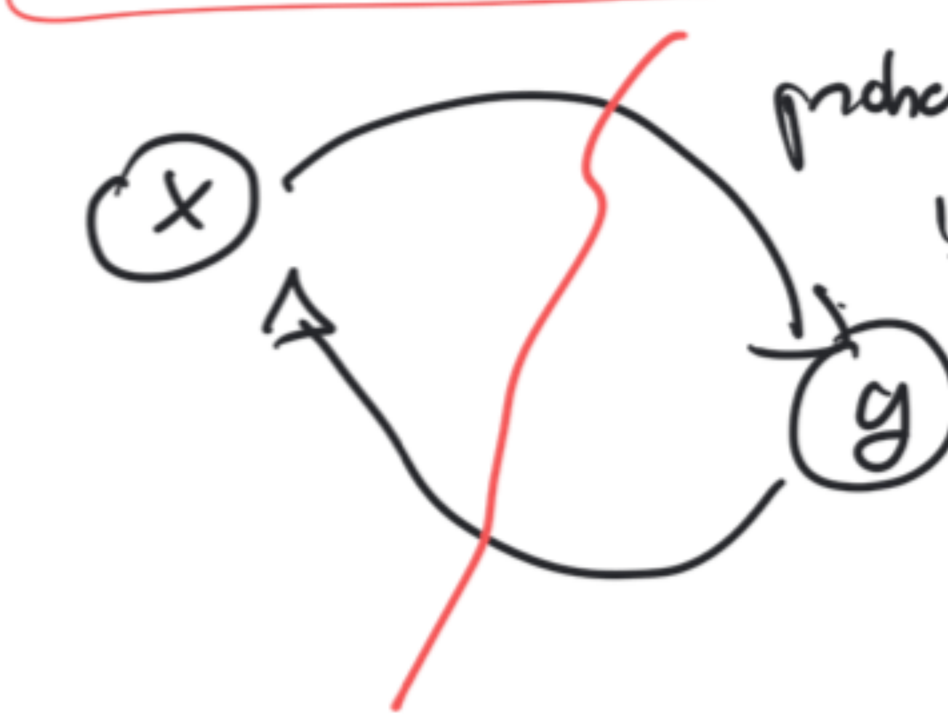
1) CONSTRUCT A DTMC s.t. $p(x)$ IS ITS steady state distribution
2) SAMPLE from $p(x)$ by SIMULATING the DTMC for "long enough" (very long single run)

Let (Π, p_0) a DTMC, p is s.s. distribution iff (Π, p_0) is ERGODIC/IRREDUCIBLE and p is invariant: $\boxed{p = p\Pi}$

$$p(x) = \sum_{y \in S} p(y) \cdot \Pi(x|y)$$

DETAILED BALANCE CONDITION

$$p(x)\Pi(y|x) = p(y)\Pi(x|y)$$



probability flow is the same in both directions at steady state

Th: $p(x)$ invariant

$$\sum_y p(x)\Pi(y|x) = \sum_y p(y)\Pi(x|y)$$

$$p(x) = \sum_y p(y)\Pi(x|y) = (p \cdot \Pi)(x) \Rightarrow p = p\Pi$$

DTMCs work also for uncountable state spaces (e.g. $\mathbb{R}$, $\mathbb{R}^n$). Call $\mathcal{X}$ is the state space.

Warning: math is harder, we ignore it, but we need to replace Π with a TRANSITION KERNEL $K(x|y)$ t.c.

1) $\forall y \in \mathcal{X}$, $K(x|y)$ is a p.d. $\int_{\mathcal{X}} K(x|y)dx = 1$, $K(x|y) \geq 0$

2) $K(x|y)$ is measurable / <u>continuous</u> wrt y

Typically, $K(x|y) = \mathcal{N}(y, \sigma^2)$!